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FRANCK-CONDON FACTORS FOR VARIOUS AIR SPECIES

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TECHNICAL REPORT NO. AFWL-TR-70-108

AIR FORCE WEAPONS LABORATORY
Air Force Systems Command
Kirtland Air Force Base
New Mexico

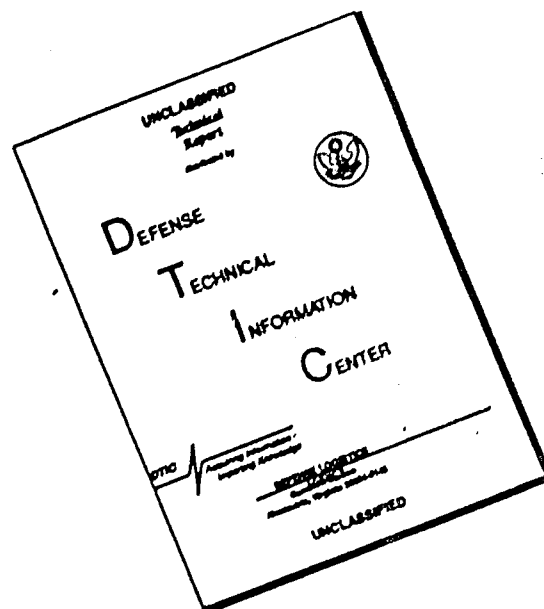
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FOREWORD

This research was performed under Program Element 61102H, Project 5710, Subtask HC 061, and was funded by the Defense Atomic Support Agency (DASA).

Inclusive dates of research were July 1967 through September 1968. The report was submitted 27 November 1970 by the Air Force Weapons Laboratory Project Officer, Captain Richard Harris (SYT).

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ABSTRACT

(Distribution Limitation Statement No. 3)

In the process of calculating opacities which are needed as input data for radiation transport problems, the absorption cross sections for various species has to be known. One factor in the cross section is the vibrational transition probability, called the Franck-Condon factor (FCF). This report presents input data needed to calculate these from Rydberg-Klein potentials as well as tables of Franck-Condon factors for species of atmospheric interest.

CONTENTS

<u>Section</u>		<u>Page</u>
I	INTRODUCTION	1
	Methods of Various Investigators	7
	Limitations of RK or RKR Methods	8
	Zare Program at AFWL	9
II	MOLECULAR SYSTEMS CONSIDERED	12
	CN (Cyanogen) Band Systems	14
	CO (Carbon Monoxide) Band Systems	18
	N ₂ (Nitrogen) Band Systems	22
	N ₂ ⁺ (Nitrogen Molecular Ion) Band Systems	26
	NO (Nitric Oxide) Band Systems	33
	O ₂ (Oxygen) Band Systems	39
	Photoionization Franck-Condon Factors	45
III	TABLES OF FRANCK-CONDON FACTORS	57
	APPENDIXES	
	I Computer Program TURNGPT	117
	II Computer Program FRANKON	143
	III Table of R-Centroids	168
	IV Additional Tables for Birge-Hopfield Tables	205
	REFERENCES	210

TABLES

<u>Table</u>		<u>Page</u>
1	Investigators Using a WKB-Type Approximation	8
2	Transitions Included	12
3	Potential Energy for the CN $X^2\Sigma^+$ State	14
4	Potential Energy for the CN $A^2\Pi_{3/2}$ State	15
5	Potential Energy for the CN $A^2\Pi_{1/2}$ State	16
6	Potential Energy for the CN $B^2\Sigma^+$ State	17
7	Additional Data Needed for CN Molecule	18
8	Potential Energy for the CO $X^1\Sigma^+$ State	19
9	Potential Energy for the CO $A^1\Pi$ State	20
10	Additional Data Needed for the CO Molecule	21
11	Potential Energy for the N_2 $X^1\Sigma_g^+$ State	21
12	Potential Energy for N_2 $A^3\Sigma_u^+$ State	22
13	Potential Energy for the N_2 $B^3\Pi_g$ State	23
14	Potential Energy for the N_2 $C^3\Pi_u$ State	24
15	Potential Energy of the N_2 $b^1\Pi_u$ State	24
16	Potential Energy of the N_2 $b'^1\Sigma_u^+$ State	25
17	Additional Data Needed for the N_2 Molecule	25
18	Molecular Data Needed for TURNPT (N_2 $b'^1\Sigma_{u1}^+$)	26
19	Molecular Data Needed for TURNPT (N_2 $b'^1\Pi_u$)	26
20	Potential Energy for the N_2^+ $X^2\Sigma_g^+$ State	27
21	Potential Energy for the N_2^+ $A^2\Pi_u$ State	28
22	Potential Energy for the N_2^+ $B^2\Sigma_u^+$ State	29
23	Potential Energy for the N_2^+ $C^2\Sigma_u^+$ State	30
24	Additional Data Needed for the N_2^+ Molecule	30
25	Molecular Data Needed for TURNPT (N_2^+ $X^2\Sigma_g^+$)	31
26	Molecular Data Needed for TURNPT (N_2^+ $B^2\Sigma_u^+$)	32

TABLES (cont'd)

<u>Table</u>		<u>Page</u>
27	Potential Energy for the NO $X^2\pi_{1/2}$ State	33
28	Potential Energy for the NO $X^2\pi_{3/2}$ State	34
29	Potential Energy for the NO $A^2\Sigma^+$ State	35
30	Potential Energy for the NO $B^2\pi$ State	36
31	Potential Energy for the NO $C^2\pi$ State	37
32	Potential Energy for the NO $B'^2\Delta$ State	37
33	Potential Energy for the NO $E^2\Sigma^+$ State	38
34	Potential Energy for the NO $D^2\Sigma^+$ State	38
35	Molecular Data Needed for TURNPT (NO $D^2\Sigma$)	39
36	Potential Energy for the O ₂ $X^3\Sigma_g^-$ State	40
37	Potential Energy for the O ₂ $B^3\Sigma_u^-$ State	41
38	Molecular Data Needed for TURNPT (O ₂ $X^3\Sigma_g^-$)	42
39	Molecular Data Needed for TURNPT (O ₂ $B^3\Sigma_u^-$)	43
40	Potential Energy Input Data Used for Calculating the Franck-Condon Factors for O ₂ Schumann-Runge Band Systems	44
41	Potential Energy for the N ₂ $X^1\Sigma_g^+$ State	46
42	Potential Energy for the N ₂ $X^2\Sigma_g^+$ State	47
43	Potential Energy for the N ₂ $A^2\pi_u$ State	48
44	Potential Energy for the N ₂ $B^2\Sigma_u^+$ State	49
45	Potential Energy for the N ₂ $C^2\Sigma_u^+$ State	50
46	Spectroscopic Constants for N ₂ Photoionization States	51
47	Potential Energy for the O ₂ $X^2\pi_g^+$ State	51
48	Potential Energy for the O ₂ $A^2\pi_u$ State	52
49	Potential Energy for the O ₂ $b^4\pi$ State	53
50	Potential Energy for the O ₂ $a^4\pi$ State	53
51	Potential Energy for the O ₂ $c^4\Sigma_u^-$ State	54
52	Potential Energy for the O ₂ $^2\Sigma_g^-$ State	55

TABLES (cont'd)

<u>Table</u>		<u>Page</u>
53	Spectroscopic Constants for O ₂ Photoionization States	55
54	RKR Franck-Condon Factors for (CN RED (1/2))	58
55	RKR Franck-Condon Factors for (CN RED (3/2))	60
56	RKR Franck-Condon Factors for (CN VIOLET)	62
57	RKR Franck-Condon Factors for (CO 4th +)	64
58	RKR Franck-Condon Factors for (N ₂ 1st +)	66
59	RKR Franck-Condon Factors for (N ₂ 2nd +)	68
60	RKR Franck-Condon Factors for (N ₂ B-H 1)	69
61	RKR Franck-Condon Factors for (N ₂ B-H 2)	71
62	RKR Franck-Condon Factors for (N ₂ + MEINEL)	73
63	RKR Franck-Condon Factors for (N ₂ + 1st Neg.)	75
64	RKR Franck-Condon Factors for (N ₂ + 2nd Neg.)	77
65	RKR Franck-Condon Factors for (NO γ (1/2))	78
66	RKR Franck-Condon Factors for (NO γ (3/2))	79
67	RKR Franck-Condon Factors for (NO β (1/2))	80
68	RKR Franck-Condon Factors for (NO β (3/2))	82
69	RKR Franck-Condon Factors for (NO δ (1/2))	84
70	RKR Franck-Condon Factors for (NO δ (3/2))	85
71	RKR Franck-Condon Factors for (NO ϵ (1/2))	86
72	RKR Franck-Condon Factors for (NO ϵ (3/2))	87
73	RKR Franck-Condon Factors for (NO β' (1/2))	88
74	RKR Franck-Condon Factors for (NO β' (3/2))	89
75	RKR Franck-Condon Factors for (NO γ' (1/2))	90
76	RKR Franck-Condon Factors for (NO γ' (3/2))	91
77	RKR Franck-Condon Factors for (NO HEATH)	92
78	RKR Franck-Condon Factors for (NO FEAST 1)	93

TABLES (cont'd)

<u>Table</u>		<u>Page</u>
79	RKR Franck-Condon Factors for (NO FEAST 2)	94
80	RKR Franck-Condon Factors for (NO E - C)	95
81	RKR Franck-Condon Factors for (NO FEAST-HEATH)	96
82	RKR Franck-Condon Factors for (NO L - M)	97
83	RKR Franck-Condon Factors for (O ₂ S - R)	98
84	RKR Franck-Condon Factors for (N ₂ PHOTO 1)	100
85	RKR Franck-Condon Factors for (N ₂ PHOTO 2)	102
86	RKR Franck-Condon Factors for (N ₂ PHOTO 3)	104
87	RKR Franck-Condon Factors for (N ₂ PHOTO 4)	106
88	RKR Franck-Condon Factors for (O ₂ PHOTO 1)	107
89	RKR Franck-Condon Factors for (O ₂ PHOTO 2)	109
90	RKR Franck-Condon Factors for (O ₂ PHOTO 3)	110
91	RKR Franck-Condon Factors for (O ₂ PHOTO 4)	111
92	RKR Franck-Condon Factors for (O ₂ PHOTO 5)	112
93	RKR Franck-Condon Factors for (O ₂ PHOTO 6)	113
94	Table of Franck-Condon Factors by Various Investigators	114
95	R-Centroids for (CN RED (1/2))	168
96	R-Centroids for (CN RED (3/2))	170
97	R-Centroids for (CN VIOLET)	172
98	R-Centroids for (CO 4th +)	174
99	R-Centroids for (N ₂ 1st +)	176
100	R-Centroids for (N ₂ 2nd +)	178
101	R-Centroids for (N ₂ B-H 1)	179
102	R-Centroids for (N ₂ B-H 2)	181
103	R-Centroids for (N ₂ + MEINEL)	183
104	R-Centroids for (N ₂ + 1st Neg.)	185

TABLES (cont'd)

<u>Table</u>		<u>Page</u>
105	R-Centroids for ($N_2 + 2nd\ Neg.$)	187
106	R-Centroids for ($NO\ \gamma\ (1/2)$)	188
107	R-Centroids for ($NO\ \gamma\ (3/2)$)	190
108	R-Centroids for ($NO\ \beta$)	192
109	R-Centroids for ($NO\ \delta\ (1/2)$)	194
110	R-Centroids for ($NO\ \delta\ (3/2)$)	195
111	R-Centroids for ($NO\ \epsilon\ (1/2)$)	196
112	R-Centroids for ($NO\ \epsilon\ (3/2)$)	197
113	R-Centroids for ($NO\ \beta'\ (1/2)$)	198
114	R-Centroids for ($NO\ \beta'\ (3/2)$)	199
115	R-Centroids for ($NO\ \gamma'$)	200
116	R-Centroids for ($NO\ FEAST\ 1$)	201
117	R-Centroids for ($NO\ FEAST\ 2$)	201
118	R-Centroids for ($NO\ FEAST-HEATH$)	202
119	R-Centroids for ($NO\ L - M$)	202
120	R-Centroids for ($O_2\ S - R$)	203
121	Spectroscopic Constants for the $N_2b'^1\Sigma_u^+$ State	206
122	Potential Energy for the $N_2b'^1\Sigma_u^+$ State	207
123	Potential Energy for the $N_2b^1\pi_u$ State	208
124	Spectroscopic Constants for the $N_2b^1\pi_u$ State	209

LIST OF VARIABLES

B_e	rotational constant in the equilibrium position
B_i	rotational constant used by Vanderslice for the i^{th} level determined by least squares fit
B_v	rotational constant for the v^{th} vibrational level
B_v^{eff}	effective rotational constant for the v vibrational level
D_e	dissociation energy of the electronic state of the molecule
dt	volume element
$E(I,K)$	vibrational-rotational energy of a molecule in terms of continuous classical variables, I,K
$E(v,J)$	vibrational-rotational energy of a molecule in terms of vibrational and rotational quantum numbers
E_R	rotational energy of a molecule
E_v	vibrational energy of a molecule
f	a Klein action integral: $\partial S / \partial U$
g	a Klein action integral: $-\partial S / \partial K$
G_v	vibrational term
$\Delta G_{v+1/2}$	separation of successive vibrational terms
\hat{H}	Hamiltonian operator
I	classical action integral, when quantized it is set equal to $h(v+1/2)$
I'	the value of I such that $U = E(I,K)$
J	rotational quantum number
K	related to classical angular momentum
l	classical angular momentum
m	mass
O_p	a general operator of quantum mechanics
p_r	linear momentum along r (internuclear separation) axis
$q_{v'v''}$	Franck-Condon factor
r	internuclear separation of molecule

LIST OF VARIABLES (cont'd)

r_e	internuclear separation at equilibrium
r_{\max}	larger of the two classical turning points
r_{\min}	smaller of the two classical turning points
$r_{v',v''}$	r centroid
$r^2_{v',v''}$	r^2 centroid
$S(U,K)$	Klein's auxiliary function
τ	total transition probability
T_e	relative energy of separation between the minimums of two electronic states
U	total vibrational-rotational energy of a molecule
U_i	energy of the i^{th} level in Vanderslice's formulation
v	vibrational quantum number
$V(r)$	rotationless vibrational potential of a molecule
V_{eff}	rotationless vibrational potential corrected for centrifugal effects
w_i	parameter in Vanderslice's formulation
α_e	rotational constant
γ_e	rotational constant
δ_e	rotational constant
ϵ_e	rotational constant
μ	reduced mass of molecule
ψ_f	final total wave function
ψ_i	initial total wave function
ψ_{fe}	final electronic wave function
ψ_{ie}	initial electronic wave function
ψ_{fR}	final rotational wave function
ψ_{iR}	initial rotational wave function
ψ_{fv}	final vibrational wave function

LIST OF VARIABLES (cont'd)

ψ_{iv}	initial vibrational wave function
ψ_v''	vibrational wave function for lower state
ψ_v'	vibrational wave function for upper state
t_v	period of vibration of molecule
w_e	vibrational constant
w_{exe}	vibrational constant
w_{eye}	vibrational constant
w_{eze}	vibrational constant
w_{ete}	vibrational constant
w_i	vibrational constant in Vanderslice's formulation determined from least squares fit
w_{ixi}	vibrational constant in Vanderslice's formulation determined from least squares fit

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SECTION I

INTRODUCTION

For any given fixed temperature, the intensity distribution of the spectrum of a band system in a typical atmospheric diatomic molecule is determined primarily by the vibrational transition probability. The intensity distribution within a vibrational band is determined by the rotational transition probability. This report will be concerned with only the calculation of the vibrational transition probabilities called the Franck-Condon factors. These are defined by the following overlap integral:

$$q_{v',v''} = \left(\int \psi_{v'} \psi_{v''} dr \right)^2 \quad (1)$$

where $\psi_{v'}$, $\psi_{v''}$ are the vibrational wave functions to be described in detail later and v' , v'' refer to the upper and lower vibrational quantum number, respectively. The Franck-Condon factors satisfy the following relations:

$$\text{all } \sum_{v'} q_{v',v''} = 1$$

and

$$\text{all } \sum_{v''} q_{v',v''} = 1 \quad (2)$$

Since the overlap integral involves the vibrational wavefunctions of the initial and final states of the molecule, the Schrodinger equation must be solved for these wavefunctions.

$$\hat{H} \psi_v = E_v \psi_v \quad (3)$$

where

ψ_v is the vibrational wavefunction of level v

E_v is the energy of vibrational level v

\hat{H} is the Hamiltonian operator for the problem

The Hamiltonian operator contains a term for the potential energy in which the two nuclei move. The correctness of this potential will determine how good the vibrational wavefunctions will be. This in turn determines the accuracy of the Franck-Condon factors. Hence the better the potential the better the Franck-Condon factors.

There have been a great many empirical potential energy functions developed over the past few decades. A study of these and the relative merits of each has been done by Steele et al. (Ref. 1).

Among the most popular potentials in the past for calculating Franck-Condon factors has been the Morse potential.

$$V(r) = D_e \left[1 - e^{-ax} \right]^2 \quad (4)$$

where

$$a = \left\{ \frac{4\pi^2 c^2 \omega_e^2 \mu}{2D_e} \right\}^{1/2}$$

D_e is the dissociation energy

$$x = (r - r_e)$$

r_e is the internuclear separation at the minimum of the potential well

r is the internuclear separation

Using this potential one can develop a closed form representation for the wavefunctions, hence the evaluation of the overlap integrals can be done without the need of a large computer. However, this potential is accurate only near the bottom of the potential well. Therefore the Franck-Condon factors for the upper vibration levels may be inaccurate.

To calculate better wavefunctions for the upper vibrational levels, one needs a better potential. One such method for calculation a better potential has been developed by Rydberg (Ref. 2) and Klein (Ref. 3), which makes use of experimentally measured data. Subsequently, it has been modified in various ways by other investigators, notably by Rees (Ref. 4). The general method has become known as the Rydberg-Klein-Rees or R-K-R method. In many instances this is a misnomer because the Rees modification is not even used.

The method is based on a WKB approximation and will be outlined below. This treatment of the basic equations is based on the derivation in a paper by Vanderslice et al. (Ref. 5).

Rydberg used two expressions from classical mechanics and modified them appropriately to obtain the corresponding quantum mechanical expressions. The classical equations for the action integral is

$$\int p_r dr = (2\mu)^{1/2} \int [\tilde{U} - \tilde{V}_{\text{eff}}]^{1/2} dr \quad (5)$$

where

p_r is the momentum in r direction

r is the internuclear separation

μ is the reduced mass of the molecule

\tilde{V}_{eff} is the effective potential

\tilde{U} is the total vibrational-rotational energy given by

$$\tilde{U} = \frac{(p_r)^2}{2\mu} + \frac{l^2}{2\mu r^2} + \tilde{V}(r) \quad (6)$$

where

l is the angular momentum of the rotating molecule

$\tilde{V}(r)$ is the potential energy of the rotationless molecule

Letting

$$K = \frac{l^2}{2\mu}$$

one then has

$$\tilde{U} = \frac{(p_r)^2}{2\mu} + \frac{K}{r^2} + \tilde{V}(r)$$

or

$$\tilde{U} = \frac{p_r^2}{2\mu} + \tilde{V}_{\text{eff}} \quad (7)$$

where

$$\tilde{V}_{\text{eff}} = \frac{K}{r^2} + \tilde{V}(r)$$

from which follows equation (7) after solving the P_r and substituting this expression in the action integral.

The action integral equation (17) is quantized as if it were a harmonic oscillator which results in the equation

$$h(v + \frac{1}{2}) = (2\mu)^{\frac{1}{2}} \int [\tilde{U} - \tilde{V}_{\text{eff}}]^{\frac{1}{2}} dr \quad (8)$$

This is the first basic equation of Rydberg's method.

The second basic equation of Rydberg involves the rotational energy of the system. Again, classically this is given by

$$\tilde{E}_r = K \left(\frac{1}{r^2} \right)_v = \frac{K}{\tau_v} \int \left(\frac{1}{r^2} \right) dt = \frac{K\mu}{\tau_v} \int \frac{1}{r^2 P_r} dr \quad (9)$$

where

K is the same as for equation (7)

τ_v is the period of vibration

Quantization of K the rotational angular momentum leads to

$$K = \frac{h^2}{8\pi^2\mu} J(J+1) \quad (10)$$

with which the rotational energy integral becomes, upon solving equation (15) for P_r and substituting this in equation (17),

$$\frac{h^2}{8\pi^2\tau} \frac{1}{\sqrt{2\mu}} \int [\tilde{U} - \tilde{V}_{\text{eff}}]^{-\frac{1}{2}} \frac{dr}{r^2} = \frac{h^2}{8\pi^2\mu} \left(\frac{1}{r^2} \right)_v = B_v \quad (11)$$

This is Rydberg's second basic equation. Rydberg solved these graphically. The second of these becomes infinite at the classical turning points since $\tilde{U} = \tilde{V}_{\text{eff}}$ there. This increases the difficulty of solving the problem graphically since large errors can be made in the regions of the classical turning points.

Klein defined a new function $S(\tilde{U}, K)$ to aid in finding the classical turning points, given by

$$S(\tilde{U}, K) = \frac{1}{(2\pi^2\nu)^{1/2}} \int_0^{I'} [\tilde{U} - \tilde{E}(I, K)]^{1/2} dI \quad (12)$$

where

$$I = h(\nu + \frac{1}{2})$$

\tilde{U} is the total energy

$$K = \frac{\hbar^2}{2\mu}$$

$\tilde{E}(I, K)$ is the vibrational-rotational energy

I' is the value of I such that $\tilde{U} = \tilde{E}(I, K)$

Using this function Klein found that expressions for the classical turning points were given by

$$\frac{\partial S}{\partial \tilde{U}} = f = \frac{1}{2} (r_{\max} - r_{\min}) \quad (13)$$

and

$$-\frac{\partial S}{\partial K} = g = \frac{1}{2} \left(\frac{1}{r_{\min}} - \frac{1}{r_{\max}} \right) \quad (14)$$

which can be inverted to give

$$r_{\min} = \left(\frac{f}{g} + f^2 \right) - f \quad (15)$$

$$r_{\max} = \left(\frac{f}{g} + f^2 \right) + f \quad (16)$$

The integration and differentiation of Klein's equations must be carried out numerically in general. Before the large computers of recent years this presented a problem. Rees therefore made the next modification to the Rydberg-Klein method, by observing that the integral for $S(\tilde{U}, K)$ could be integrated analytically if in the function $\tilde{E}(I, K)$, I is expressible as a quadratic (or cubic) form in $(\nu + \frac{1}{2})$. Consequently, f, g can be written in closed form.

Vanderslice et al. capitalized on this observation and have fitted the energy $\tilde{E}(I, K)$ with a series of quadratics over the whole energy range of the potential function. They then obtained a closed form representation for g, f

and consequently, r_{\min} and r_{\max} . Their expressions for g and f are

$$f = \left(\frac{h}{8\pi^2 \mu c} \right)^{1/2} \sum_{i=1}^n (wx)_i^{-1/2} \ln W_i \quad (17)$$

$$g = \left(\frac{2\pi^2 \mu c}{h} \right)^{1/2} \sum_{i=1}^n \left[\frac{1}{2} \alpha_i (wx)_i^{-1} \left(U_i^{1/2} - U_{i-1}^{1/2} \right) + (wx)_i^{-1/2} \left(2B_i - \alpha_i (wx)_i^{-1} W_i \right) \ln W_i \right] \quad (18)$$

where

$$W_i = \left[\frac{W_i^2 - 4(wx)_i U_i}{W_i^2 - 4(wx)_i U_{i-1}} \right]^{1/2} \left[\frac{W_i - 2(wx)_i^{1/2} U_{i-1}^{1/2}}{W_i - 2(wx)_i^{1/2} U_i^{1/2}} \right] \quad (19)$$

W_i is the coefficient of $(v+1/2)$

wx_i is the coefficient of $(v+1/2)^2$

α_i is the coefficient of $(v+1/2) J(J+1)$ (coupling constant)

β_i is the coefficient of $J(J+1)$

Vanderslice et al. also give a simple interpretation of the $S(\tilde{U}, K)$ function of Klein. $S(\tilde{U}, K)$ is one half the area between the constant total energy curve, \tilde{U} , and the potential curve $V_{\text{eff}}(r)$ (see figure 1).

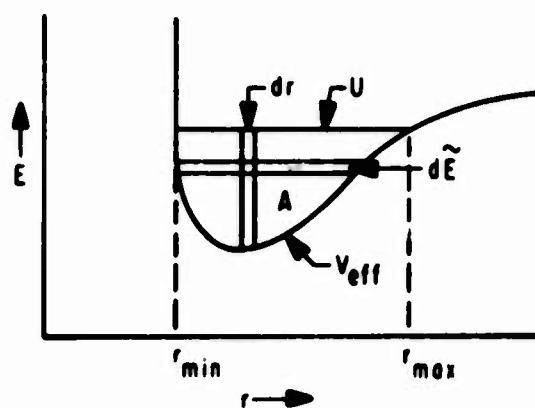


Figure 1. Interpretation of the Klein S Function

Following Vanderslice,

$$dI = \tau dE \quad (20)$$

with

$$\tau = \left(\frac{\mu}{2}\right)^{1/2} \int (E - V_{\text{eff}})^{-1/2} dr \quad (21)$$

putting τdE in for dI in Klein's equation for S ,

$$S(\tilde{U}, K) = \frac{1}{(2\pi^2\mu)^{1/2}} \int_0^I [\tilde{U} - \tilde{E}(I, K)]^{1/2} dI$$

one finds,

$$S = \frac{1}{2\pi} \int_0^U (\tilde{U} - \tilde{E})^{1/2} \left[(\tilde{E} - \tilde{V}_{\text{eff}})^{-1/2} d\tilde{r} \right] d\tilde{E}$$

or

$$S = \frac{1}{2\pi} dr \int_{V_{\text{eff}}}^U (\tilde{U} - \tilde{E})^{1/2} (\tilde{E} - \tilde{V}_{\text{eff}})^{1/2} d\tilde{E} \quad (22)$$

The lower limit of the second integral is V_{eff} since it is evaluated at a constant value of r .

The last integral becomes, after some manipulation,

$$S = \frac{1}{2} \int_{r_{\text{min}}}^{r_{\text{max}}} dr \int_{V_{\text{eff}}}^U dE = \frac{1}{2} A \quad (23)$$

1. METHODS OF VARIOUS INVESTIGATORS

Many investigators have reported calculating RKR potentials for molecules of importance in heated air. Table 1 contains the name of the investigator (or investigators) and the general method used.

Table 1

INVESTIGATORS USING A WKB-TYPE APPROXIMATION

<u>Name</u>	<u>Method</u>
Flinn, Spindler, Fifer	RKR
Gilmore	RK, KDJ
Ginter, Battino	RKR
Halmann, Laulicht	RK
Jarmain	KDJ
Jain, Shani, Singh	RKR
Krupenie, Weissman	RK
Richards, Barrow	RK-RKR (hybrid)
*Vanderslice et al.	RKR
Zare, Albritton	RK
AFWL	RK

The RK method uses Klein's equations and numerically integrates them in some fashion. The RKR method uses the quadratic fit of Rees in some fashion. The KDJ method makes use of a series developed by Jarmain (Ref. 6) based on a series expansion of a WKB approximation by Dunham (Ref. 7). With some simplifying approximations this expansion is the same as a series expansion of Klein's equations, which are also based on a WKB approximation. Hurley (Ref. 8) has shown the two methods are equivalent and can be deduced from the same basic equation.

2. LIMITATIONS OF RK OR RKR METHODS

Ginter and Battino (Ref. 9) have discussed the effects of experimental errors and errors due to approximations made in the formulation of equations used in the RKR methods on the calculated potential curves. A summary of their conclusions will be presented.

*Co-author with several people on different papers.

The accuracy with which one can represent the vibrational-rotational energy levels of an electronic state of a diatomic molecule by a polynomial $E(v,J)$ primarily determines the accuracy of the calculated potential. The errors in determining $E(v,J)$ fall into three categories:

- (1) Experimental error in spectroscopic data
- (2) Error caused by fitting the best polynomial $E(v,J)$ to the spectroscopic data
- (3) Error caused by fitting the spectroscopic data to a particular form of $E(v,J)$

From (1) there can be errors because of uncertainty in determining B_v^{eff} and ΔG and errors due to using the effective constants directly. From (2) often times the experimental data will fit with any one of several expansions and do it equally well. From (3) if a series of expansions of quadratic form for $E(v,J)$ is assumed, then errors may be introduced because of the fitting of local fluctuations in the experimental data.

3. ZARE PROGRAM AT AFWL

Several years ago R. N. Zare made available to the Air Force Weapons Laboratory (AFWL) a set of computer programs needed to construct R-K molecular potentials for diatomic molecules and to calculate Franck-Condon factors, r-centroids, and relative intensities from these potentials. A summary of the methods of the programs will be given.

The molecular potential generation program is one which was written by J. Kasper (Ref. 10). The equations,

$$f = \frac{h}{2\pi(2\mu)^{1/2}} \int_0^{I'} [U - E(I,K)]^{-1/2} dI \quad (24)$$

$$g = \frac{h}{2\pi(2\mu)^{1/2}} \int_0^{I'} B_v [U - E(I,K)]^{-1/2} dI \quad (25)$$

are integrated directly without assuming an analytic form for the integral near the upper limit.

For the energy $E(I,K)$ of the level of interest either the conventional expansion

$$\begin{aligned} \bar{E}(v,J) = & \omega_e(v+\frac{1}{2}) - \omega_e x_e(v+\frac{1}{2})^2 + \omega_e y_e(v+\frac{1}{2})^3 \\ & + \omega_e z_e(v+\frac{1}{2})^4 + \omega_e t_e(v+\frac{1}{2})^5 + \dots \\ & + B_v J(J+1) - D_v J^2(J+1)^2 + \dots \end{aligned} \quad (26)$$

or the G_v, B_v obtained directly from the spectroscopic data can be used. The variables I, K are of course related to v, J by

$$I = h(v+\frac{1}{2}) \quad (27)$$

$$K = \frac{h^2}{2\pi^2\mu} J(J+1) \quad (28)$$

From the f, g the values of r_{\min} and r_{\max} are calculated for each vibrational level. These are then used as input data to the Franck-Condon factor program. To calculate the wavefunctions needed in the Franck-Condon factor program, the radial Schrodinger equation is solved (for the wavefunctions) by a numerical method developed by Cooley (Ref. 11). The one-dimensional second order Schrodinger equation,

$$\frac{d^2}{dr^2} \psi + [E(v,J) - V_{\text{eff}}(r,J)] \psi = 0 \quad (29)$$

where

$E(v,J)$ is the energy of the particular level,

$$V_{\text{eff}}(r,J) = V(r) + \frac{h^2}{8\pi^2\mu r^2} J(J+1) \quad (30)$$

is the energy of rotationless level corrected for rotation, and ψ , the vibration-rotation wavefunction, is changed to a finite difference equation.

The finite difference equation is solved iteratively for $E(v,J)$ the eigenvalue and ψ the eigenfunction, until the $E(v,J)$ and the previous $E(v,J)$ differ by an arbitrarily small amount. The wavefunctions thus obtained are used in the evaluation of the square of the overlap integral which is the Franck-Condon factor.

$$q_{v',v''} = \int \psi_{v',J'} \psi_{v'',J''} dr^2 \quad (31)$$

They are also used in evaluating the r-centroids.

$$r_{v',v''} = \frac{\int \psi_{v'} r \psi_{v''} dr}{\int \psi_{v'} \psi_{v''} dr} \quad (32)$$

$$r_{v',v''}^2 = \frac{\int \psi_{v'} r^2 \psi_{v''} dr}{\int \psi_{v'} \psi_{v''} dr} \quad (33)$$

The integrals are all evaluated using a Simpson's rule numerical integration procedure. The relative intensities scaled to ten are also calculated.

The programs provided by Dr. Zare have been adapted for use on the AFWL CDC 6600 computer. Since this computer carries 15 decimal numbers per word, the double precision subroutines were removed. The (v',v'') array size for the computed Franck-Condon factor was increased to (20,23). Some of the input statements were modified and output statements were added. Aside from these changes the program used at AFWL is the same as the one developed and used by Dr. Zare.

SECTION II

MOLECULAR BAND SYSTEMS CONSIDERED

The motivation for calculating Franck-Condon factors at AFWL is their use in calculating transition strengths of diatomic molecules. These strengths are used in part to calculate absorption coefficients which in turn are frequency averaged over prechosen frequency groups to give opacities for air. These opacities are desired over a large temperature density range. When determining which molecules are candidates for inclusion in the opacity calculation, one must take into account the chemistry that goes on in this heated air. After picking the potential molecules one looks at the various transitions allowed in the molecules and the relative strengths and positions (in energy) of the transitions. Then from these one arrives at a list of important electronic band systems of diatomic molecules in heated air.

The following table contains information on all transitions considered in the present work. The transition involved, common name of the band system, the source of the potential, and array size calculated are listed.

Table 2

TRANSITIONS INCLUDED

<u>States involved</u>	<u>Name</u>	<u>Source of potential</u>		<u>Array size (v'v'')</u>
		<u>Upper</u>	<u>Lower</u>	
CN $B^2\Sigma^+ - CN X^2\Sigma^+$	CN violet	13	13	(18,18)
CN $A^2\Pi_{1/2} - CN X^2\Sigma^+$	CN red	13	13	(18,18)
CN $A^2\Pi_{3/2} - CN X^2\Sigma^+$	CN red	13	13	(18,18)
CO $A^1\Pi - CO X^1\Sigma^+$	CO 4th positive	16	16	(20,24)
N ₂ $B^3\Pi_g - N_2 A^3\Sigma_u^+$	1st positive	18	18	(17,13)
N ₂ $C^3\Pi_u - N_2 B^3\Pi_g$	2nd positive	18	18	(4,17)
N ₂ $b'^1\Sigma_u^+ - N_2 X^1\Sigma_g^+$	Birge-Hopfield #1	33	19	(20,21)
N ₂ $b'^1\Pi_u - N_2 X^1\Sigma_g^+$	Birge-Hopfield #2	33	19	(24,21)

Table 2 (cont'd)

States involved	Name	Source of potential		Array size (v'v'')
		Upper	Lower	
$N_2^+ A^2 \pi_u - N_2^+ X^2 \Sigma_g^+$	Meinel	33	33	(20,20)
$N_2^+ B^2 \Sigma_u^+ - N_2^+ X^2 \Sigma_g^+$	1st negative	33	33	(20,20)
$N_2^+ C^2 \Sigma_u^+ - N_2^+ X^2 \Sigma_g^+$	2nd negative	33	33	(10,20)
$NO A^2 \Sigma^+ - NO X^2 \pi_{1/2}$	γ (gamma)	22	23	(5,23)
$NO A^2 \Sigma^+ - NO X^2 \pi_{3/2}$	γ (gamma)	22	23	(5,23)
$NO B^2 \pi - NO X^2 \pi_{1/2}$	β (beta)	22	23	(19,23)
$NO B^2 \pi - NO X^2 \pi_{3/2}$	β (beta)	22	23	(19,23)
$NO C^2 \pi - NO X^2 \pi_{1/2}$	δ (delta)	22	23	(4,23)
$NO C^2 \pi - NO X^2 \pi_{3/2}$	δ (delta)	22	23	(4,23)
$NO D^2 \Sigma^+ - NO X^2 \pi_{1/2}$	ϵ (epsilon)	33	23	(7,23)
$NO D^2 \Sigma^+ - NO X^2 \pi_{3/2}$	ϵ (epsilon)	33	23	(7,23)
$NO B'^2 \Delta_1 - NO X^2 \pi_{1/2}$	β' (beta prime)	22	23	(5,23)
$NO B'^2 \Delta_1 - NO X^2 \pi_{3/2}$	β' (beta prime)	22	23	(5,23)
$NO E^2 \Sigma^+ - NO X^2 \pi_{1/2}$	γ' (gamma prime)	22	23	(5,23)
$NO E^2 \Sigma^+ - NO X^2 \pi_{3/2}$	γ' (gamma prime)	22		(5,23)
$NO G^2 \Sigma - NO X^2 \pi_{1/2}$	Lagergrist-Miescher	33	23	(7,23)
$NO C^2 \pi - NO A^2 \Sigma^+$	Heath	22	22	(4,5)
$NO D^2 \Sigma^+ - NO A^2 \Sigma^+$	Feast 1	22	22	(7,5)
$NO E^2 \Sigma^+ - NO A^2 \Sigma^+$	Feast 2	22	22	(5,5)
$NO E^2 \Sigma^+ - NO C^2 \pi$		22	22	(5,4)
$NO E^2 \Sigma^+ - NO D^2 \Sigma^+$	Feast-Heath	22	33	(5,7)
$O_2 B^3 \Sigma_u^- - O_2 X^3 \Sigma_g^-$	Schumann-Runge	33	33	(20,23)
	$N_2 - N_2^+$			
$N_2 X^1 \Sigma_g^+ - N_2^+ X^2 \Sigma_g^+$	1st	33	33	(20,20)

Table 2 (cont'd)

States involved	Name	Source of potential		Array size (v'v'')
		Upper	Lower	
$N_2 \ X^1\Sigma_g^+ - N_2^+ \ A^2\Pi_u$	2nd	33	33	(20,20)
$N_2 \ X^1\Sigma_g^+ - N_2^+ \ B^2\Sigma_u^+$	3rd	33	33	(20,20)
$N_2 \ X^1\Sigma_g^+ - N_2^+ \ C^2\Sigma_u^+$	4th	33	33	(10,20)
$O_2 - O_2^+$				
$O_2 \ X^3\Sigma_g^- - O_2^+ \ X^2\Pi_g$	1st	33	33	(14,23)
$O_2 \ X^3\Sigma_g^- - O_2^+ \ a^4\Pi_u$	2nd	33	33	(10,23)
$O_2 \ X^3\Sigma_g^- - O_2^+ \ A^2\Pi_u$	3rd	33	33	(10,23)
$O_2 \ X^3\Sigma_g^- - O_2^+ \ b^4\Sigma_g^-$	4th	33	33	(10,23)
$O_2 \ X^3\Sigma_g^- - O_2^+ \ ^2\Sigma_g^-$	5th	33	33	(10,23)
$O_2 \ X^3\Sigma_g^- - O_2^+ \ c^4\Sigma_u^-$	6th	33	33	(10,23)

1. CN (CYANOGEN) BAND SYSTEMS

The potentials used to calculate Franck-Condon factors were taken from the paper by Fallon, Vanderslice, and Cloney (Ref. 13). Tables 3 through 6 contain the data for the potential energy curves for the various CN states used.

Table 7 contains other molecular data needed by the FRANKON program.

Table 3*

POTENTIAL ENERGY FOR THE CN $X^2\Sigma^+$ STATE

v	$V(\text{cm}^{-1})$	r_{\min}	r_{\max}	$V(\text{ev})$
0	1031.1	1.1237	1.2244	0.1278
1	3073.6	1.0923	1.1676	0.3811
2	5089.7	1.0722	1.2997	0.6310
3	7079.5	1.0566	1.3274	0.8777
4	9042.8	1.0438	1.3525	1.1211
5	10980.0	1.0327	1.3760	1.3613
6	12890.0	1.0230	1.3984	1.5981

Table 3* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
7	14775.0	1.0143	1.4198	1.8317
8	16632.0	1.0063	1.4406	2.0620
9	18463.0	0.9991	1.4610	2.2890
10	20267.0	0.9924	1.4809	2.5127
11	22045.0	0.9861	1.5005	2.7330
12	23797.0	0.9803	1.5200	2.0503
13	25520.0	0.9749	1.5393	3.1639
14	27217.0	0.9696	1.5583	3.3743
15	28887.0	0.9648	1.5774	3.5813
16	30530.0	0.9602	1.5964	3.7850
17	32146.0	0.9558	1.6153	3.9853
18	33734.0	0.9516	1.6343	4.1823

*Reference 13.

Table 4*

POTENTIAL ENERGY FOR THE CN A²π_{3/2} STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	903.99	1.1827	1.2900	0.1121
1	2691.1	1.1482	1.3354	0.3336
2	4452.9	1.1269	1.3701	0.5521
3	6189.4	1.1105	1.4001	0.7673
4	7900.4	1.0969	1.4273	0.9795
5	9585.0	1.0852	1.4529	1.1884
6	11245.0	1.0749	1.4773	1.3942
7	12880.0	1.0657	1.5007	1.5968

Table 4* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
8	14487.0	1.0573	1.5236	1.7960
9	16070.0	1.0477	1.5459	1.9923
10	17627.0	1.0526	1.5679	2.1853
11	19158.0	1.0360	1.5896	2.3751
12	20663.0	1.0298	1.6111	2.5617
13	22142.0	1.0240	1.6325	2.7451
14	23594.0	1.0186	1.6538	2.9254
15	25021.0	1.0134	1.6750	3.1020
16	26422.0	1.0083	1.6960	3.2757
17	27795.0	1.0038	1.7175	3.4460
18	29142.0	0.9994	1.7388	3.6130

*Reference 13.

Table 5*

POTENTIAL ENERGY FOR THE CN A² $\pi_{1/2}$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	903.99	1.1816	1.2891	0.1121
1	2691.1	1.1484	1.3356	0.3336
2	4452.9	1.1272	1.3704	0.5521
3	6189.4	1.1109	1.4006	0.7673
4	7900.4	1.0975	1.4280	0.9795
5	9585.9	1.0860	1.4527	1.1884
6	11245.0	1.0759	1.4783	1.3942
7	12880.0	1.0668	1.5019	1.5968
8	14487.0	1.0587	1.5249	1.7960
9	16070.0	1.0512	1.5475	1.9923

Table 5* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
10	17627.0	1.0443	1.5696	2.1853
11	19158.0	1.0379	1.4916	2.3751
12	20663.0	1.0319	1.6133	2.5617
13	22142.0	1.0263	1.6348	2.7451
14	23594.0	1.0211	1.6563	2.9254
15	25021.0	1.0161	1.6778	3.1020
16	26422.0	1.0115	1.6992	3.2757
17	27795.0	1.0070	1.7207	3.4460
18	29142.0	1.0028	1.7423	3.6130

*Reference 13.

Table 6*

POTENTIAL ENERGY FOR THE CN B²Σ⁺ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1077.0	1.104	1.203	0.1335
1	3200.0	1.074	1.246	0.3968
2	5284.0	1.055	1.279	0.6551
3	7325.0	1.040	1.307	0.9081
4	9321.0	1.027	1.333	1.1556
5	11269.0	1.016	1.358	1.3971
6	13167.0	1.007	1.383	1.6324
7	15011.0	0.999	1.407	1.8611
8	16799.0	0.992	1.432	2.0827
9	18527.0	0.986	1.457	2.2969
10	20192.0	0.980	1.483	2.5034

Table 6* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
11	21795.0	0.974	1.509	2.7021
12	23338.0	0.970	1.535	2.8933
13	24821.0	0.965	1.562	3.0773
14	26249.0	0.961	1.589	3.2542
15	27623.0	0.957	1.617	3.4247
16	28948.0	0.953	1.644	3.5889
17	30228.0	0.950	1.672	3.7475
18	31464.0	0.946	1.701	3.9008

*Reference 13.

Table 7

ADDITIONAL DATA NEEDED FOR THE CN MOLECULE

<u>State</u>	<u>De</u>	<u>Be</u>	<u>ae</u>	<u>ye</u>	<u>Te</u>
X ² Σ ⁺	61525.88	1.8996	0.01735	0	0.0
A ² π _{3/2}	52279.86	1.7165	0.01746	0	9222.04
A ² π _{1/2}	52279.86	1.7165	0.01746	0	9272.62
B ² Σ ⁺	54774.34	1.9701	0.02215	0	25752.4

2. CO (CARBON MONOXIDE) BAND SYSTEMS

The only band of CO considered to be of possible importance in absorption in heated air is the CO 4th positive system. The potentials used in calculating the Franck-Condon factors were taken from the paper by Krupenie and Weisman (Ref. 16). Tables 8 and 9 contain the data for the potential curves of the lower and upper states. Table 10 contains other molecular data needed by the program.

Table 8*

POTENTIAL ENERGY FOR THE CO $X^1\Sigma^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1081.590	1.083	1.179	0.1341
1	3224.864	1.053	1.220	0.3998
2	5341.654	1.034	1.250	0.6623
3	7432.026	1.020	1.276	0.9214
4	9496.948	1.008	1.300	1.1773
5	11533.76	0.997	1.322	1.4300
6	13545.20	0.988	1.343	1.6794
7	15530.64	0.980	1.363	1.9255
8	17489.9	0.972	1.383	2.1684
9	19423.5	0.965	1.402	2.4081
10	21330.7	0.959	1.420	2.6446
11	23212.4	0.953	1.438	2.8779
12	25068.5	0.947	1.456	3.1080
13	26898.4	0.942	1.474	3.3349
14	28703.2	0.937	1.492	3.5587
15	30482.7	0.932	1.509	3.7793
16	32235.4	0.928	1.526	3.9966
17	33963.9	0.923	1.544	4.2109
18	35666.8	0.919	1.561	4.4220
19	37344.4	0.916	1.579	4.6300
20	38997.5	0.912	1.596	4.9349
21	40625.7	0.908	1.614	5.0368
22	42208.0	0.905	1.631	5.2330
23	43776.0	0.901	1.649	5.4274

*Reference 16.

Table 9*

POTENTIAL ENERGY FOR THE CO $A^2\Pi$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	753.49	1.183	1.297	0.0934
1	2242.3	1.148	1.348	0.2780
2	3685.1	1.126	1.387	0.4569
3	5097.9	1.110	1.422	0.6320
4	6476.1	1.096	1.454	0.8029
5	7818.2	1.085	1.484	0.9693
6	9125.0	1.075	1.514	1.1313
7	10401.8	1.066	1.542	1.2896
8	11641.0	1.058	1.571	1.4433
9	12846.9	1.051	1.599	1.5928
10	14018.8	1.044	1.627	1.7381
11	15155.6	1.038	1.656	1.8790
12	16262.0	1.031	1.685	2.0162
13	17333.0	1.027	1.714	2.1490
14	18371.0	1.022	1.743	2.2777
15	19366.0	1.017	1.773	2.4010
16	20330.0	1.013	1.804	2.5205
17	21257.0	1.009	1.837	2.6355
18	22138.0	1.005	1.871	2.7447
19	22970.0	1.001	1.090	2.8478
20	23762.0	0.996	1.051	2.9460

*Reference 16.

Table 10*

ADDITIONAL DATA NEEDED FOR THE CO MOLECULE

$$(\mu = 6.85841)$$

<u>State</u>	<u>De</u>	<u>Be</u>	<u>ae</u>	<u>ye</u>	<u>Te</u>
$X^1\Sigma^+$	89597.4	1.93127	0.617513	2.960E-6	0.0
$A^1\Pi$	24522.8	1.226	0.018	0.0	133740.0

*Gilmore, DASA Handbook 1917 old copy Volume I tables.

3. N_2 (NITROGEN) BAND SYSTEMS

The potentials used to calculate the Franck-Condon factors for the nitrogen systems came from several sources. The $X^1\Sigma_g^+$, $A^3\Sigma_u^+$, $B^3\Pi_u$, and $C^3\Pi_u$ states contained in tables 11 through 14 were taken from the paper by Benesch et al. (Ref. 18). The potentials used for the $b^1\Pi_u$ and $b'^1\Sigma_u^+$ states were generated at AFWL with program TURNGPT and are listed in tables 15 and 16, respectively. The data for the $b^1\Pi_u$ state are from Lofthus (Ref. 19) and the data for the $b'^1\Sigma_u^+$ state are from Wilkinson (Ref. 20). These data are listed in tables 17 through 18.

Table 11*

POTENTIAL ENERGY FOR THE N_2 $X^1\Sigma_g^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>V(ev)</u>
0	1175.5	1.055 ₀	1.145 ₆	0.14573
1	3505.2	1.026 ₆	1.184 ₃	0.42456
2	5806.5	1.008 ₃	1.213 ₀	0.71987
3	8079.2	0.994 ₂	1.237 ₇	1.00163
4	10323.3	0.982 ₆	1.260 ₀	1.27985
5	12538.8	0.972 ₅	1.280 ₉	1.55452
6	14725.4	0.963 ₆	1.300 ₇	1.82561

Table 11* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>V(ev)</u>
7	16883.1	0.955 ₆	1.319 ₇	2.09311
8	19011.8	0.948 ₄	1.338 ₂	2.35702
9	21111.5	0.941 ₇	1.356 ₁	2.61733
10	23182.0	0.935 ₅	1.373 ₈	2.87403
11	25223.3	0.929 ₈	1.391 ₁	3.12710
12	27235.3	0.924 ₄	1.408 ₂	3.37654
13	29218.0	0.919 ₄	1.425 ₂	3.62235
14	31171.2	0.914 ₆	1.442 ₀	3.86450
15	33094.9	0.910 ₁	1.458 ₈	4.10300
16	34989.0	0.905 ₈	1.475 ₅	4.33782
17	36853.5	0.901 ₇	1.492 ₁	4.56898
18	38688.3	0.897 ₈	1.508 ₈	4.79645
19	40493.4	0.894 ₀	1.525 ₅	5.02024
20	42268.6	0.890 ₄	1.542 ₃	5.24032
21	44014.1	0.887 ₀	1.559 ₁	5.45672

*Reference 18.

Table 12*

POTENTIAL ENERGY FOR THE N₂ A³Σ_u⁺ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>V(ev)</u>
0	726.80	1.2329	1.3482	0.0901
1	2159.67	1.1979	1.3992	0.2678
2	3564.87	1.1758	1.4378	0.4420
3	4942.36	1.1589	1.4715	0.6127
4	6292.03	1.1450	1.5025	0.7801
5	7613.75	1.1332	1.5319	0.9439

Table 12* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>V(ev)</u>
6	8907.33	1.1229	1.5602	1.1043
7	10172.54	1.1138	1.5877	1.2612
8	11409.10	1.1055	1.6149	1.4145
9	12616.69	1.0980	1.6417	1.5642
10	13794.95	1.091 ₁	1.668 ₅	1.7103
11	14943.47	1.084 ₇	1.695 ₃	1.8526
12	16061.80	1.078 ₇	1.722 ₂	1.9913
13	17149.44	1.073 ₂	1.749 ₃	2.1261

*Reference 18.

Table 13*

POTENTIAL ENERGY FOR THE N₂ B³π_g STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>V(ev)</u>
0	863.16	1.1631	1.2689	0.10702
1	2568.14	1.1306	1.3150	0.31840
2	4244.46	1.1099	1.3497	0.52623
3	5891.92	1.0940	1.3798	0.73049
4	7510.38	1.0809	1.4074	0.93114
5	9099.74	1.0697	1.4334	1.12819
6	10659.92	1.0599	1.4583	1.32163
7	12190.86	1.0511	1.4825	1.51144
8	13692.50	1.0432	1.5061	1.69761
9	15164.76	1.0360	1.5294	1.88014
10	16607.54	1.0294	1.5524	2.05902
11	18020.70	1.0233	1.5753	2.23422
12	19404.04	1.0176	1.5981	2.40573

Table 13* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>V(ev)</u>
13	20757.31	1.012 ₃	1.621 ₀	2.57351
14	22080.16	1.007 ₄	1.644 ₀	2.73752
15	23372.16	1.002 ₇	1.667 ₂	2.89770
16	24632.76	0.998 ₂	1.690 ₆	3.05399
17	25861.32	0.994 ₀	1.714 ₃	3.20631

*Reference 18.

Table 14*

POTENTIAL ENERGY FOR THE N₂ C³π_u STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>V(ev)</u>
0	1016.71	1.1030	1.2005	0.12605
1	3011.11	1.0730	1.2438	0.37332
2	4951.90	1.0540	1.2771	0.61394
3	6825.93	1.0395	1.3076	0.84629
4	8607.21	1.0282	1.3388	1.06713

*Reference 18.

Table 15*

POTENTIAL ENERGY OF THE N₂ b¹π_u STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	412.5	1.23007	1.38773	0.0511
1	1114.5	1.16992	1.45950	0.1381
2	1779.5	1.13007	1.51097	0.2206
3	2407.5	1.09562	1.55852	0.2984
4	2992.5	1.06450	1.60407	0.3710

Table 15* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
5	3546.5	1.03665	1.64718	0.4396
6	4062.5	1.00840	1.69329	0.5036
7	4542.4	0.98508	1.73570	0.5631

*From TURNGPT using Lofthus data.

Table 16*

POTENTIAL ENERGY OF THE N₂ b'¹Σ_u⁺ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	374.6	1.36740	1.52792	0.0464
1	1116.6	1.31442	1.59394	0.1384
2	1848.9	1.38936	1.65220	0.2292
3	2571.6	1.25162	1.68331	0.3188
4	3284.7	1.22812	1.72036	0.4072
5	3988.2	1.20746	1.75474	0.4944
6	4682.0	1.18887	1.78724	0.5804

*From TURNGPT using Wilkinson data.

Table 17

ADDITIONAL DATA NEEDED FOR THE N₂ MOLECULE

<u>State</u>	<u>De</u>	<u>Be</u>	<u>ae</u>	<u>ye</u>	<u>Te</u>
X ¹ Σ _g ⁺	78717.0	1.9987	0.0178	0.0	0.0
A ³ Σ _u ⁺	28499.0	1.4545	0.01794	-9.2 x 10 ⁻⁵	50218.0
B ³ Π _u	38306.0	1.6375	0.01794	-7.4 x 10 ⁻⁵	59639.0
C ³ Π _u	28643.0	1.8259	0.0197	0.0	69302.0

Table 17 (cont'd)

<u>State</u>	<u>De</u>	<u>Be</u>	<u>ae</u>	<u>ye</u>	<u>Te</u>
$b^1\pi_u$	55655.0*	1.154	0.0048	0.0	104473.0
$b^1\Sigma_u^+$	55655.0*	---	---	---	102288.0

*Estimated value.

Table 18

MOLECULAR DATA NEEDED FOR TURNGPT ($N_2 \ b^1\Sigma_{u1}^+$)

<u>State</u>	<u>We</u>	<u>Wexe</u>	<u>Weye</u>	<u>Weze</u>	<u>Be</u>	<u>ae</u>	<u>ye</u>	<u>re</u>
$b^1\Sigma_u^+$	751.64	4.82	0	0	1.154	0.0048	0	1.4443

Table 19

MOLECULAR DATA NEEDED FOR TURNGPT ($N_2 \ b^1\pi_u$)

<u>v</u>	<u>Gv</u>	<u>Bv</u>
0	0	1.41
1	702	1.41
2	1367	1.40
3	1995	1.41
4	2580	1.48
5	3134	1.47
6	3650	---

4. N_2^+ (NITROGEN MOLECULAR ION) BAND SYSTEMS

The potentials used to generate the Franck-Condon factors for the N_2^+ band systems were calculated with program TURNGPT. The $A^2\pi_u$ and $C^2\Sigma_u^+$ states were generated using spectroscopic constants given by Gilmore (Ref. 21). These are given in table 24. The $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$ states were generated by using spectroscopic data from Lofthus (Ref. 19). These data are listed in tables 25 and 26. The B_v for the missing levels was obtained by graphical interpolation. The

generated potentials are listed in tables 20 through 23.

Table 20*

POTENTIAL ENERGY FOR THE $N_2^+ X^2\Sigma_g^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
0	1099.4	1.07794	1.1664
1	3274.2	1.04341	1.20672
2	5416.4	1.02546	1.23763
3	7525.8	1.01122	1.26388
4	9602.2	0.99944	1.28783
5	11645.4	0.97947	1.20991
6	13654.4	0.97947	1.33082
7	15630.1	0.97184	1.35192
8	17570.0	0.96441	1.37203
9	19477.0	0.95803	1.39205
10	21349.0	0.95185	1.41160
11	23185.9	0.94604	1.43092
12	24987.0	0.94066	1.45022
13	26751.8	0.93552	1.46943
14	28479.9	0.93092	1.48894
15	30171.0	0.92638	1.50835
16	31824.5	0.92239	1.52823
17	33439.9	0.91853	1.54825
18	35016.7	0.91482	1.56848
19	36554.0	0.91152	1.58931
20	38051.7	0.90810	1.61014

*From Lofthus data.

Table 21*

POTENTIAL ENERGY FOR THE $N_2^+ A^2\Pi_u$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	947.96	1.02650	1.22743	0.1175
1	2821.38	1.09570	1.27158	0.3498
2	4664.80	1.07615	1.30488	0.5783
3	6478.22	1.06118	1.33368	0.8031
4	8271.64	1.04887	1.38479	1.0242
5	10015.06	1.03838	1.38479	1.2416
6	11738.48	1.02917	1.40847	1.4553
7	13431.90	1.02097	1.43137	1.6652
8	15095.32	1.01357	1.45371	1.8714
9	16728.74	1.00681	1.47563	2.0739
10	18332.16	1.00061	1.40726	2.2727
11	19905.58	0.99487	1.51867	2.4678
12	21449.00	0.98954	1.53995	2.6791
13	22962.42	0.98455	1.56116	2.8468
14	24445.84	0.97987	1.58235	3.0307
15	25897.26	0.97546	1.60356	3.2109
16	27322.68	0.97130	1.62484	3.3880
17	28716.10	0.967356	1.64622	2.5601
18	30079.52	0.96361	1.66774	3.7291
19	31412.94	0.96003	1.68943	3.8944
20	32716.36	0.95662	1.71132	4.0560

*From Gilmore's constants.

Table 22*

POTENTIAL ENERGY FOR THE $N_2^+ B^2\Sigma_u^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1197.15	1.03331	1.12304	0.1484
1	3588.66	1.00546	1.16196	0.4424
2	5887.46	0.98795	1.19199	0.7299
3	9147.86	0.97409	1.21811	1.0101
4	10344.26	0.96323	1.24330	1.2824
5	12467.06	0.95501	1.26903	1.5456
6	14508.06	0.94720	1.27401	1.7986
7	16459.16	0.94043	1.32000	2.0405
8	18291.36	0.93404	1.34765	2.2677
9	20018.26	0.92856	1.37643	2.4818
10	21614.96	0.92315	1.40798	2.6797
11	23094.86	0.91867	1.44118	2.8632
12	24466.26	0.91496	1.117632	3.0332
13	25742.56	0.91145	1.51208	3.1914
14	26938.86	0.90846	1.54832	3.3397
15	28065.46	0.90544	1.58452	3.4794
16	29132.56	0.90303	1.62095	3.6117
17	30148.06	0.90104	1.65763	3.7376
18	31114.06	0.89893	1.69439	3.8574
19	32036.06	0.89687	1.73160	3.9717
20	32858.06	0.89012	1.78474	4.0736

*From Lofthus data.

Table 23*

POTENTIAL ENERGY FOR THE $N_2^+ C^2\Sigma_u^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1034.08	1.21465	1.31124	0.1282
1	3085.06	1.18158	1.34967	0.3824
2	5111.94	1.15962	1.37772	0.6337
3	7113.28	1.14238	1.40182	0.8818
4	9087.64	1.12798	1.42383	1.1266
5	11033.58	1.11558	1.44462	1.3679
6	12949.66	1.10471	1.46470	1.6054
7	14832.44	1.09508	1.48437	1.8391
8	16686.48	1.08646	1.50386	2.0687
9	18504.34	1.07874	1.52333	2.2941
10	20286.58	1.07182	1.54294	2.5150

*From Gilmore's constants

Table 24

ADDITIONAL DATA NEEDED FOR THE N_2^+ MOLECULE

<u>State</u>	<u>We</u>	<u>Wexe</u>	<u>Weye</u>	<u>Weze</u>	<u>WeTe</u>	<u>Te</u>
$X^2\Sigma_g^+$	2207.17	16.146	-2.85×10^{-2}	9.2×10^{-4}	0	0.0
$A^2\Pi_u$	1903.42	15.0	0.0	0.0	0	8219.6
$B^2\Sigma_u^+$	2418.7	22.53	-6.70×10^{-1}	4.0×10^{-2}	0	25461.6
$C^2\Pi_u$	2073	10.97	-2.40×10^{-1}	0.0	0	64607.5
<u>State</u>	<u>Be</u>	<u>ae</u>	<u>ye</u>	<u>de</u>	<u>re</u>	
$X^2\Sigma_g^+$	1.9258	0.01743	-1.64×10^{-4}	0	1.118	
$A^2\Pi_u$	1.748	0.02	0.00	0	1.117	
$B^2\Sigma_u^+$	2.083	0.0183	-1.65×10^{-3}	0	1.075	
$C^2\Sigma_u^+$	1.5124	0.0017	-7.50×10^{-4}	0	1.262	

Table 25

MOLECULAR DATA NEEDED FOR TURNPT $\left(N_2^+ X^2\Sigma_g^+\right)$

\underline{v}	$\underline{G_v}$	$\underline{B_v}$
0	1099.4	1.922
1	3274.2	1.902
2	5416.4	1.879
3	7525.8	1.861
4	9602.2	1.841
5	11645.2	1.826
6	13654.4	1.808
7	15630.1	1.781
8	17570.0	1.766
9	19477.0	1.740
10	21349.1	1.724
11	23185.9	1.703
12	24987.0	1.683
13	26751.8	1.663
14	28479.9	1.639
15	30171.0	1.620
16	31824.5	1.593
17	33439.9	1.572
18	35016.7	1.548
19	36554.0	1.522
20	38051.7	1.500

Table 26

MOLECULAR DATA NEEDED FOR TURNPT $N_2^+ B^2\Sigma_u^+$

<u>v</u>	<u>Gv</u>	<u>Bv</u>
0	1197.16	2.073
1	3568.66	2.049
2	5887.46	2.025
3	8147.86	2.002
4	10344.26	1.968
5	12467.06	1.926
6	14508.06	1.896
7	16459.16	1.896
8	18291.36	1.81
9	20018.26	1.761
10	21614.06	1.710
11	23094.86	1.653
12	24466.26	1.595
13	25742.56	1.545
14	26938.86	1.494
15	28065.46	1.452
16	29132.56	1.404
17	30148.06	1.361
18	31114.06	1.323
19	32036.06	1.285
20	32858.06	1.250

5. NO (NITRIC OXIDE) BAND SYSTEMS

The molecular potentials used to calculate the various NO band system Franck-Condon factors came from three sources. The $X^2\pi_{1/2}$, $X^2\pi_{3/2}$ states were from Vanderslice (Ref. 23). The $A^2\Sigma^+$, $B^2\pi$, $C^2\pi$, $B'^2\Delta$, $E^2\Sigma^+$ states were from Vanderslice et al. (Ref. 22). The NO $D^2\Sigma^+$ state potential was generated with program TURNGPT using molecular constants from Gilmore (Ref. 21). The potentials are listed in tables 27 through 34. The spectroscopic constants used to generate the D state potential are listed in table 35.

Table 27*

POTENTIAL ENERGY FOR THE NO $X^2\pi_{1/2}$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	948.5	1.202	1.105	0.1176
1	2825.0	1.245	1.074	0.3503
2	4673.0	1.276	1.055	0.5795
3	6493.0	1.304	1.041	0.8051
4	8285.0	1.329	1.028	1.027
5	10048.0	1.352	1.018	1.246
6	11784.0	1.375	1.009	1.461
7	13492.0	1.396	1.000	1.673
8	15172.0	1.417	0.993	1.881
9	16824.0	1.438	0.986	2.086
10	18448.0	1.458	0.974	2.388
11	20044.0	1.478	0.980	2.485
12	21613.0	1.497	0.974	2.680
13	23152.0	1.517	0.968	2.871
14	24665.0	1.537	0.963	3.058
15	26149.0	1.556	0.958	3.131
16	27605.0	1.576	0.954	3.423
17	29034.0	1.596	0.945	3.600

Table 27* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
18	30434.0	1.615	0.941	3.774
19	31805.0	1.636	0.937	3.944
20	33141.0	1.656	0.934	4.109
21	34443.0	1.677	0.930	4.271
22	35714.0	1.698	0.926	4.418
23	36953.0	1.719	0.923	4.582

*Reference 23.

Table 28*

POTENTIAL ENERGY FOR THE NO X² $\pi_{3/2}$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	948.5	1.204	1.106	0.1176
1	2825.0	1.246	1.076	0.3503
2	4673.0	1.278	1.057	0.5795
3	6493.0	1.305	1.042	0.8051
4	8285.0	1.330	1.030	1.027
5	10048.0	1.354	1.019	1.246
6	11784.0	1.376	1.010	1.461
7	13492.0	1.397	1.002	1.673
8	15172.0	1.418	0.994	1.881
9	16824.0	1.439	0.987	2.086
10	18448.0	1.459	0.981	2.288
11	20044.0	1.479	0.975	2.485
12	21613.0	1.499	0.969	2.680
13	23152.0	1.518	0.964	2.871

Table 28* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
14	24663.0	1.538	0.959	3.058
15	26145.0	1.558	0.955	3.242
16	27599.0	1.577	0.950	3.422
17	29024.0	1.597	0.946	3.599
18	30423.0	1.617	0.942	3.772
19	31790.0	1.637	0.938	3.942
20	33124.0	1.657	0.934	4.107
21	34424.0	1.678	0.930	4.269
22	35695.0	1.698	0.926	4.426
23	36938.0	1.719	0.923	4.580

*Reference 23.

Table 29*

POTENTIAL ENERGY FOR THE NO A²Σ⁺ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	1183.0	1.109	1.022	0.1467
1	3525.0	1.147	0.995	0.4371
2	5835.0	1.175	0.977	0.7235
3	8111.0	1.199	0.964	1.006
4	10354.0	1.220	0.953	1.284
5	12564.0	1.242	0.943	1.558

*Reference 23.

Table 30*

POTENTIAL ENERGY OF THE NO B² π STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	516.8	1.488	1.356	0.0641
1	1540.0	1.545	1.315	0.191
2	2549.0	1.588	1.289	0.316
3	3545.0	1.625	1.269	0.440
4	4519.0	1.658	1.253	0.560
5	5492.0	1.690	1.239	0.681
6	6447.0	1.719	1.226	0.799
7	7390.0	1.748	1.215	0.917
8	8323.0	1.776	1.205	1.032
9	9238.0	1.804	1.196	1.146
10	10144.0	1.831	1.188	1.258
11	11030.0	1.857	1.180	1.368
12	11911.0	1.883	1.173	1.477
13	12772.0	1.909	1.167	1.584
14	13609.0	1.935	1.161	1.688
15	14463.0	1.962	1.154	1.793
16	15293.0	1.989	1.147	1.896
17	16081.0	2.015	1.142	1.994
18	16859.0	2.041	1.136	2.091
19	17612.0	2.068	1.130	2.184

*Reference 23.

Table 31*

POTENTIAL ENERGY OF THE NO $C^2\pi$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	1194.0	1.109	1.022	0.1481
1	3556.0	1.148	0.997	0.4409
2	5922.0	1.178	0.981	0.7343
3	8192.0	1.204	0.970	1.016
4	10491.0	1.228	0.961	1.301

*Reference 23.

Table 32*

POTENTIAL ENERGY OF THE NO $B'^2\Delta$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	604.0	1.368	1.246	0.07493
1	1789.0	1.424	1.209	0.2219
2	2943.0	1.466	1.186	0.3649
3	4062.0	1.503	1.168	0.5037
4	5177.0	1.539	1.153	0.6420
5	6212.0	1.570	1.139	0.7703

*Reference 23.

Table 33*

POTENTIAL ENERGY OF NO $E^2\Sigma^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	1183.0	1.112	1.025	0.1467
1	3525.0	1.150	0.997	0.4371
2	5835.0	1.177	0.980	0.7235
3	8114.0	1.202	0.966	1.006
4	10360.0	1.223	0.955	1.285
5	12575.0	1.244	0.945	1.559

*Reference 23.

Table 34*

POTENTIAL ENERGY FOR THE NO $D^2\Sigma^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1156.336	1.02039	1.10891	0.1433
1	3438.004	0.99320	1.14762	0.4262
2	5687.031	0.97601	1.17645	0.7050
3	7918.479	0.97601	1.20099	0.9817
4	10152.686	0.96318	1.22264	1.2586
5	12415.274	0.94545	1.24187	1.5392
6	14737.141	0.93970	1.25881	1.8270
7	17154.469	0.93579	1.27350	2.1267

*From TURNGPT using Gilmore's constants

Table 35

MOLECULAR DATA NEEDED FOR TURNGPT (NO $D^2\Sigma$)

<u>We</u>	<u>We_e</u>	<u>We_y</u>	<u>We_z</u>	<u>Be</u>	<u>ae</u>	<u>ye</u>	<u>re</u>
2323.9	22.885	0.75	0.22	2.0026	2.175×10^{-2}	0	1.062

6. O₂ (OXYGEN) BAND SYSTEM

Franck-Condon factors were calculated for only the O₂ Schumann-Runge band system. The potentials needed, O₂ X³Σ and O₂ B³Σ, were calculated with program TURNGPT using data from Wallace (Ref. 24). The G, ΔG, B_v were each plotted and the best smooth curve was drawn through these. These smoothed values were then used as input data to TURNGPT. The B³Σ state was found to have a hook near the dissociation limit on the inner branch of the potential curve. This is similar to the findings of many other investigators, for example, Vanderslice et al. (Ref. 25), F. Gilmore (Ref. 26), Richards and Barrow (Ref. 27),* Ginter, Battino (Ref. 28).

A potential which is not single valued causes numerical difficulties when one attempts to find solutions for the wave functions needed to calculate overlap integrals. To avoid this problem the calculated potential for the B³Σ state was used up to the vibrational level where the hook started to occur. First an extrapolation of the form a/r^{12} was used. (This procedure is similar to that used by Halmann and Laulicht (Ref. 29) who used Vanderslice's potential for their calculations.) Using the resulting potential to find the maximum of the Schumann-Runge continuum by the reflection method, one finds that it occurs at a much too high energy. An alternate method for constructing a more realistic potential in the troublesome region involves using the calculated potential at values of vibrational quantum number where one believes the calculation and using Evans and Schexander's (Ref. 30) values for the potential in the continuum portion of the potential and interpolating through the troublesome region. Franck-Condon factors were calculated using the so determined potentials.

*They claim no anomaly though.

Table 36*

POTENTIAL ENERGY FOR THE $O_2 \ X^3\Sigma_g^-$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
0	789.81	1.15966	1.26310
1	2352.20	1.12759	1.30786
2	3891.68	1.10739	1.34156
3	5408.25	1.09177	1.37059
4	6901.91	1.07892	1.39709
5	8372.64	1.06791	1.42192
6	9820.43	1.05849	1.44586
7	11245.26	1.04980	1.46867
8	12647.12	1.04186	1.49078
9	14025.99	1.03482	1.51266
10	15381.88	1.02825	1.53410
11	16714.79	1.02215	1.55527
12	18024.69	1.01657	1.56737
13	19311.59	1.01136	1.59734
14	20575.48	1.00645	1.61823
15	21816.33	1.00183	1.63910
16	23034.10	0.99764	1.66018
17	21228.74	0.99367	1.68130
18	25400.22	0.98988	1.70249
19	26548.54	0.98618	1.72369
20	27673.62	0.98325	1.74566
21	28775.15	0.97498	1.76236
22	29852.56	0.97249	1.78501
23	30905.29	0.97124	1.80913

*From TURNGPT

Table 37*

POTENTIAL ENERGY FOR THE O_2 $B^3\Sigma_u^-$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
0	353.45	1.52754	1.68252
1	1041.45	1.46883	1.75912
2	1706.55	1.45786	1.81448
3	2347.95	1.43628	1.86469
4	2965.55	1.41890	1.91241
5	3557.35	1.40495	1.96052
6	4118.45	1.39306	2.00873
7	4651.65	1.37998	2.05627
8	5153.05	1.36959	2.01829
9	5618.55	1.36125	2.16443
10	6047.45	1.35429	2.22607
11	6435.65	1.34833	2.29561
12	6781.05	1.34334	2.37479
13	7081.75	1.33902	2.46677
14	7336.75	1.33507	2.57613
15	7545.15	1.33088	2.70806
16	7714.11	1.32861	2.86245
17	7847.02	1.32627	3.04965
18	7949.15	1.32496	3.27710
19	8024.79	1.32740	3.56375
20	8077.44	1.33034	3.94952

*From TURNGPT

Table 38

MOLECULAR DATA NEEDED FOR TURNPT ($O_2 \times^3\Sigma^-_g$)

<u>v</u>	<u>Gv(cm⁻¹)</u>	<u>Bv(cm⁻¹)</u>
0	789.81	1.4375
1	2352.20	1.4215
2	3891.68	1.406
3	5408.25	1.3909
4	6901.91	1.3755
5	8372.64	1.3601
6	9820.43	1.343
7	11245.26	1.3296
8	12647.12	1.3145
9	14026.00	1.298
10	15381.88	1.2833
11	16714.79	1.2678
12	18024.69	1.2516
13	19311.59	1.236
14	20575.48	1.2204
15	21816.33	1.2046
16	23034.10	1.1870
17	24228.74	1.1711
18	25400.22	1.1550
19	26548.54	1.1390
20	27673.62	1.1226
21	28775.15	1.640
22	29852.56	1.0904
23	30905.29	1.0744

Table 39

MOLECULAR DATA NEEDED FOR TURNINGPT ($O_2 \ B^3\Sigma_u^-$)

<u>v</u>	<u>Gv(cm⁻¹)</u>	<u>Bv(cm⁻¹)</u>
0	353.45	0.813
1	1041.45	0.798
2	1706.55	0.785
3	2347.95	0.770
4	2965.55	0.754
5	3557.35	0.735
6	4118.45	0.719
7	4652.65	0.703
8	5153.05	0.680
9	5618.55	0.655
10	6047.45	0.627
11	6435.65	0.596
12	6781.05	0.562
13	7081.75	0.525
14	7336.75	0.485
15	7545.15	0.443
16	7714.11	0.398
17	7847.02	0.354
18	7949.15	0.306
19	8024.79	0.258
20	8077.44	0.208
21	8109.38	0.159
22	8126.28	0.109

Table 39 (cont'd)

CONTINUUM VALUES

9150.0	1.31
9560.0	1.305
9970.0	1.300
10380.0	1.295
10780.0	1.290
11200.0	1.285
11640.0	1.28

Table 40

POTENTIAL ENERGY INPUT DATA USED FOR CALCULATING THE FRANCK-CONDON
FACTORS FOR O₂ SCHUMANN-RUNGE BAND SYSTEMS

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
0	353.45	1.52754	1.68252
1	1041.45	1.46883	1.75912
2	1706.55	1.45786	1.81448
3	2347.95	1.43628	1.86469
4	2965.55	1.41890	1.91241
5	3557.35	1.40495	1.96052
6	4118.45	1.39306	2.00873
7	4652.65	1.37998	2.05627
8	5153.05	1.36959	2.10829
9	5618.55	1.36125	2.16443
10	6047.45	1.35429	2.22607
11	6435.65	1.34833	2.29561
12	6781.05	1.34334	2.37479
13	7081.75	1.33902	2.46677
14	7336.75	1.33507	2.57613

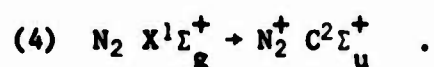
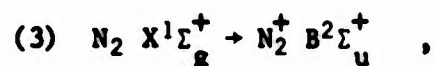
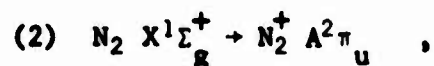
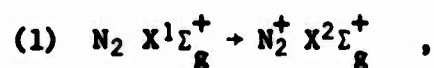
Table 40 (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
15	7545.15	---	2.70806
16	7714.11	---	2.86245
17	7847.02	---	3.04965
18	7949.15	---	3.27710
19	8024.79	---	3.56375
20	8077.44	---	3.94952

7. PHOTOIONIZATION FRANCK-CONDON FACTORS

a. N₂

The four photoionization transitions considered were



All five potentials used were generated using program TURNPT and with the exception of the B state were generated from spectroscopic constants given by Gilmore (Ref. 21). The B state was generated by use of constants from Herzberg (Ref. 29).

Table 46 contains the spectroscopic data used. Tables 41 through 45 contain the generated potentials.

Table 41*

POTENTIAL ENERGY FOR THE $N_2 \ X^1\Sigma_g^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
0	1175.49	1.05485	1.14544
1	3505.14	1.02644	1.18417
2	5806.91	1.06820	1.21288
3	8078.91	0.99410	1.23755
4	10322.88	0.98242	1.25993
5	12538.14	0.97236	1.28081
6	14724.61	0.96349	1.30064
7	16882.22	0.95552	1.31968
8	19010.90	0.94829	1.33813
9	21110.57	0.94164	1.35612
10	23181.15	0.93550	1.37375
11	25222.58	0.92978	1.39111
12	27234.78	0.92443	1.40825
13	39317.67	0.91940	1.42522
14	31171.18	0.91464	1.44208
15	33095.24	0.91014	1.45884
16	34989.77	0.90586	1.47556
17	36854.69	0.90178	1.49224
18	38689.94	0.89788	1.50893
19	40495.43	0.89415	1.152564
20	52271.10	0.89056	1.54240

*From TURNGPT using Gilmore's constants.

Table 42*

POTENTIAL ENERGY FOR THE $N_2^+ X^2\Sigma_g^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
0	1099.54	1.07397	1.16768
1	3274.34	1.04461	1.20792
2	5416.60	1.02575	1.23791
3	7526.22	1.01120	1.26385
4	9603.09	0.99917	1.28752
5	11647.12	0.98884	1.30976
6	13658.25	0.97978	1.33100
7	15636.45	0.97170	1.35156
8	17581.70	0.96440	1.37161
9	19494.00	0.95777	1.39130
10	21373.38	0.95169	1.41075
11	23219.89	0.94611	1.43002
12	25033.61	0.94096	1.44919
13	26814.62	0.93619	1.46831
14	28563.05	0.93178	1.48743
15	30279.03	0.92768	1.50659
16	31962.72	0.92389	1.52582
17	33614.31	0.92037	1.54515
18	35233.99	0.91712	1.56462
19	36822.00	0.91412	1.58424
20	38378.58	0.91136	1.60404

*From TURNGPT using Gilmore's constants.

Table 43*

POTENTIAL ENERGY FOR THE N_2^+ $A^2\pi_u$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	947.96	1.02656	1.22743	0.1175
1	2821.38	1.09570	1.27158	0.3498
2	4664.80	1.07615	1.30488	0.5783
3	6478.22	1.06118	1.33368	0.8031
4	8271.64	1.04887	1.38479	1.0242
5	10015.06	1.03838	1.38479	1.2416
6	11738.48	1.02917	1.40847	1.4553
7	13431.90	1.02097	1.43137	1.6652
8	15095.32	1.01357	1.45371	1.8714
9	16728.74	1.00681	1.47563	2.0739
10	18332.16	1.00061	1.49726	2.2727
11	19905.58	0.99487	1.51867	2.4678
12	21449.00	0.98954	1.53995	2.6791
13	22962.42	0.98455	1.56116	2.8468
14	24445.84	0.97987	1.58235	3.0307
15	25897.26	0.97546	1.60356	3.2109
16	27322.68	0.97130	1.62484	3.3880
17	28716.10	0.967356	1.64622	3.5601
18	30079.51	0.96361	1.66774	3.7291
19	31412.94	0.96003	1.68943	3.8944
20	32716.36	0.95662	1.71132	4.0560

*From TURNGPT using Gilmore's constants.

Table 44

POTENTIAL ENERGY FOR THE $N_2^+ B^2\Sigma_u^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1197.15	1.03331	1.12304	0.1484
1	3588.66	1.00546	1.16196	0.4424
2	5887.46	0.98795	1.19199	0.7299
3	8147.86	0.97409	1.21811	1.0101
4	10344.26	0.96323	1.24330	1.2824
5	12467.06	0.95501	1.26903	1.5456
6	14508.06	0.94720	1.27401	1.7986
7	16469.16	0.94043	1.32000	2.0405
8	18291.36	0.93404	1.34765	2.2677
9	20018.26	0.92856	1.37643	2.4818
10	21614.96	0.92315	1.40798	2.6797
11	23094.86	0.91867	1.44118	2.8632
12	24466.26	0.91496	1.117632	3.0332
13	25742.56	0.91145	1.51208	3.1914
14	26938.86	0.90846	1.54832	3.3397
15	28065.46	0.90544	1.58452	3.794
16	29132.56	0.90303	1.62095	3.6117
17	30148.06	0.90104	1.65763	3.7376
18	31114.06	0.89893	1.69439	3.8574
19	32036.06	0.89687	1.73160	3.9717
20	32858.06	0.89012	1.78474	4.0736

Table 45*

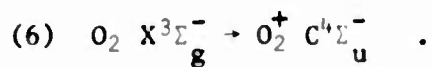
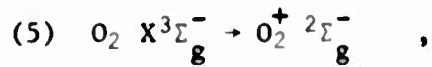
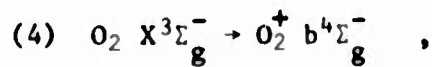
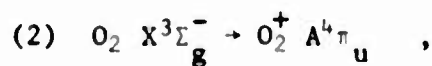
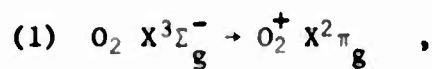
POTENTIAL ENERGY FOR THE $N_2^+ C^2\Sigma_u^+$ STATE

v	$V(\text{cm}^{-1})$	r_{\min}	r_{\max}	$V(\text{ev})$
0	1034.08	1.21465	1.31124	0.1282
1	3085.06	1.18158	1.34967	0.3824
2	5111.94	1.15962	1.37772	0.6337
3	7113.28	1.14238	1.49182	0.8818
4	9087.64	1.12798	1.42383	1.1266
5	11033.58	1.11558	1.44462	1.3679
6	12949.66	1.10471	1.46470	1.6054
7	14832.44	1.09508	1.48437	1.8391
8	16686.48	1.08646	1.50386	2.0687
9	18504.34	1.07874	1.52333	2.2941
10	20286.58	1.07182	1.54294	2.5150

*From TURNGPT using Gilmore's constants.

b. O_2

The photoionization transitions considered were



The seven potentials used were generated by program TURNPT. The $O_2 X^3\Sigma_g^-$ state was generated by using data from Wallace (Ref. 24). This is the same potential that was used as the lower state of the O_2 S-R system. The six states of O_2^+ were all generated using the spectroscopic constants given by Gilmore (Ref. 21). These data are listed in table 53. The potentials are listed in tables 47 through 52.

Table 46

SPECTROSCOPIC CONSTANTS FOR N_2 PHOTOIONIZATION STATES

<u>We</u>	<u>Wexe</u>	<u>Weye</u>	<u>Weze</u>	<u>Be</u>	<u>ae</u>	<u>ye</u>	<u>re</u>
<u>$N_2 X^1\Sigma_g^+$ state</u>							
2358.07	14.188	-1.24^{-2}	0.0	1.9987	0.0178	0.0	1.0976
<u>$N_2^+ X^2\Sigma_g^+$ state</u>							
2207.17	16.146	-2.85^{-2}	9.2^{-4}	1.9258	0.01743	-1.64^{-4}	1.118
<u>$N_2^+ A^2\Pi_u$ state</u>							
1903.42	15.0	0.0	0.0	1.748	0.02	0.0	1.117
<u>$N_2^+ B^2\Sigma_u^+$ state</u>							
2418.7	22.53	-6.7^{-1}	4.0^{-2}	2.083	0.0183	-1.65^{-3}	1.075
<u>$N_2^+ C^2\Sigma_u^+$ state</u>							
2073.7	10.97	-2.4^{-1}	0.0	1.5124	0.0017	-7.5^{-4}	1.262

Table 47*

POTENTIAL ENERGY FOR THE $O_2^+ X^2\Pi_g$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	934.12	1.07839	1.17354	0.1158
1	2777.56	1.04947	1.21552	0.3444
2	2587.94	1.03116	1.247.4	0.5678
3	6365.26	1.01714	1.26466	0.7891
4	8109.52	1.00561	1.29990	1.0054

Table 47* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
5	9820.72	0.99575	1.32370	1.2175
6	11498.86	0.98710	1.34652	1.4256
7	13143.94	0.97939	1.36865	1.6295
8	14755.96	0.97241	1.39030	1.8294
9	16334.92	0.96603	1.41161	2.0252
10	17880.82	0.96016	1.43268	2.2168
11	19393.66	0.95471	1.45362	2.4044
12	20873.44	0.94962	1.47448	2.5878
13	22320.16	0.94484	1.49534	2.7672
14	23733.82	0.94034	1.51624	2.9424

*From TURNPT using Gilmore's constants.

Table 48*

POTENTIAL ENERGY FOR THE O₂⁺ A²Π_u STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	446.08	1.34603	1.48386	0.0553
1	1317.68	1.30607	1.54794	0.1634
2	2161.88	1.28114	1.59762	0.2680
3	2978.68	1.26225	1.64192	0.3695
4	3768.08	1.24682	1.68348	0.4672
5	4530.08	1.23364	1.72353	0.5616
6	5246.68	1.22209	1.76277	0.6505
7	5971.88	1.21173	1.80167	0.7404
8	6651.88	1.20230	1.84057	0.8246
9	7304.08	1.19358	1.87975	0.9055
10	7929.08	1.08541	1.91945	0.9830

*From TURNPT using Gilmore's constants.

Table 49*

POTENTIAL ENERGY FOR THE $O_2^+ b^4\pi$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	594.11	1.22498	1.34439	0.0736
1	1756.70	1.19030	1.39967	0.2178
2	2885.11	1.16869	1.44240	0.3577
3	3979.34	1.15234	1.48038	0.4933
4	5099.39	1.13900	1.51592	0.6248
5	6065.26	1.12765	1.55006	0.7520
6	7056.95	1.11772	1.58341	0.8749
7	8014.46	1.10886	1.61637	0.9936
8	8937.79	1.10082	1.64922	1.1081
9	9826.94	1.09343	1.68218	1.2183
10	10681.91	1.08656	1.71545	1.3243

*From TURNGPT using Gilmore's constants.

Table 50*

POTENTIAL ENERGY FOR THE $O_2^+ a^4\pi$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	515.25	1.32207	1.45020	0.0639
1	1530.05	1.28390	1.50774	0.1897
2	2425.29	1.25993	1.55142	0.3130
3	3497.64	1.24174	1.58969	0.4336
4	4450.21	1.22690	1.62500	0.5517
5	5382.00	1.21429	1.65846	0.6672
6	6293.01	1.20332	1.69071	0.7802
7	7183.24	1.19358	1.72214	0.8906

Table 50* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
8	8052.60	1.18484	1.75304	0.9983
9	8901.36	1.17690	1.78360	1.1036
10	9729.25	1.16963	1.81397	1.2062

*From TURNGPT using Gilmore's constants.

Table 51*

POTENTIAL ENERGY FOR THE O₂⁺ c⁴Σ_u⁻ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1195.50	1.14677	1.23086	0.1482
1	3559.50	1.12238	1.26895	0.4413
2	5887.50	1.10740	1.29783	0.7299
3	8079.50	1.09628	1.32307	1.0141
4	10435.50	1.08740	1.34627	1.2938
5	12655.50	1.08006	1.368916	1.8390
6	14839.50	1.07383	1.28917	1.8398
7	16987.50	1.06847	1.40954	2.1060
8	19099.50	1.06382	1.42945	2.3679
9	21175.50	1.05974	1.44904	2.6253
10	23215.50	1.05916	1.46839	2.8782

*From TURNGPT using Gilmore's constants.

Table 52*

POTENTIAL ENERGY FOR THE $O_2^+ \Sigma_g^-$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	360.50	1.28272	1.43501	0.0447
1	1066.50	1.23627	1.50491	0.1322
2	1752.50	1.20657	1.55759	0.2173
3	2418.50	1.18361	1.60411	0.2998
4	3064.50	1.16440	1.64740	0.3799
5	3690.50	1.14791	1.68880	0.4575
6	4296.50	1.13310	1.72910	0.5327
7	4882.50	1.11970	1.76878	0.6053
8	5448.50	1.10730	1.80821	0.6755
9	5994.50	1.09572	1.84768	0.7432
10	6520.50	1.08478	1.88740	0.8084

*From TURNGPT using Gilmore's constants.

Table 53

SPECTROSCOPIC CONSTANTS FOR O_2 PHOTOIONIZATION STATES

<u>We</u>	<u>Wexe</u>	<u>Weye</u>	<u>Weze</u>	<u>Be</u>	<u>oe</u>	<u>ye</u>	<u>re</u>
<u>$O_2^+ X^2\Pi_g$ state</u>							
1876.50	16.53	0	0	1.67220	0.01984	0.0	1.12270
<u>$O_2^+ a^4\Pi_u$ state</u>							
1035.69	10.39	0	0	1.10461	0.01575	0.0	1.38126
<u>$O_2^+ A^2\Pi_u$ state</u>							
899.00	13.70	0	0	1.06170	0.01906	-1.95 ⁻⁴	1.40890
<u>$O_2^+ b^4\Sigma_g^-$ state</u>							
1196.77	17.09	0	0	1.28729	0.02206	0.0	1.27953

Table 53 (cont'd)

<u>We</u>	<u>Wexe</u>	<u>Weye</u>	<u>Weze</u>	<u>Be</u>	<u>ae</u>	<u>ye</u>	<u>re</u>
				<u>$O_2^+ \ ^2\Sigma_g^-$ state</u>			
726.00	10.00	0	0	1.15000	0.01700	0.0	estimated
				<u>$O_2^+ \ c^4\Sigma_g^-$ state</u>			
2400.00	18.00	0	0	1.50000	0.02000	0.0	estimated

SECTION III

TABLES OF FRANCK-CONDON FACTORS

This section contains tables of the Franck-Condon factors calculated from the data given in Section II. In Appendix I is a listing of program TURNPT which was used to generate the input data for program FRANKON. The Franck-Condon factors have been calculated by program FRANKON which is listed in Appendix II.

Table 94 contains a list of R-K-R Franck-Condon factor tabulations known to the authors at the time this work was started. This list includes only transitions of interest for atmospheric diatomic molecules.

Table 54

RKR FRANCK-CONDON FACTORS FOR CIV RED (1/2)

v'	v''	1	2	3	4	5	6	7	8	9
0	4.991-1	3.719-1	1.104-1	1.702-2	1.409-3	5.354-3	1.774-3	5.030-3	1.307-3	6.022-1-
1	3.190-1	4.573-2	3.532-1	2.222-1	5.312-2	5.253-3	3.096-4	1.293-3	3.122-7	2.201-3
2	1.258-1	2.387-1	1.208-2	2.145-1	2.884-1	1.030-1	1.513-2	1.250-2	5.327-5	1.124-0
3	4.022-2	1.333-1	9.735-2	9.004-2	9.621-2	2.933-1	1.591-1	3.230-2	3.064-3	1.453-4
4	1.154-2	9.494-2	1.793-1	1.467-2	1.554-1	1.453-2	2.552-1	2.014-1	5.411-2	6.267-3
5	3.127-3	3.532-2	1.330-1	1.197-1	2.353-3	1.533-1	1.150-3	2.040-1	2.465-1	8.174-2
6	8.362-4	1.255-2	6.343-2	1.390-1	5.541-2	3.277-2	1.259-1	2.634-2	1.346-1	2.646-1
7	2.184-4	4.950-3	2.919-2	9.517-2	1.173-1	1.272-2	7.305-2	7.756-2	6.735-2	7.238-2
8	5.060-5	1.245-3	1.118-2	4.377-2	1.034-1	7.335-2	3.044-3	1.014-1	3.289-2	1.049-1
9	1.409-5	3.734-4	3.347-3	2.234-2	5.903-2	1.045-1	4.093-2	1.175-2	1.056-1	5.984-3
10	3.807-6	1.104-4	1.350-3	9.142-3	3.674-2	9.350-2	8.590-2	1.259-2	3.599-2	9.040-2
11	1.052-6	3.252-5	4.501-4	3.533-3	1.722-2	5.187-2	8.753-2	5.957-2	4.544-4	6.026-2
12	3.004-7	9.733-6	1.470-4	1.315-3	7.423-3	2.759-2	6.435-2	8.123-2	3.269-2	4.001-3
13	9.037-8	2.377-6	4.838-5	4.775-4	3.075-3	1.342-2	3.921-2	7.159-2	6.622-2	1.188-2
14	2.816-8	9.402-7	1.598-5	1.709-4	1.227-3	5.101-3	2.123-2	5.011-2	7.191-2	4.637-2
15	8.738-9	3.053-7	5.353-6	6.051-5	4.771-4	2.550-3	1.050-2	3.020-2	5.000-2	6.484-2
16	2.575-9	1.007-7	1.822-6	2.156-5	1.824-4	1.117-3	5.115-3	1.659-2	3.928-2	6.137-2
17	6.820-10	3.258-8	6.226-7	7.717-6	5.943-5	4.503-4	2.293-3	8.542-3	2.376-2	4.692-2
18	1.519-10	9.979-9	2.088-7	2.760-6	2.595-5	1.952-4	1.010-3	4.131-3	1.327-2	3.125-2

Table 54 (cont'd)

CM RED (1/2)

V	VV	10	11	12	13	14	15	15	17	19
6	2.760-11	9.355-11	2.139-12	0.749-12	3.332-12	3.903-12	2.534-12	6.120-12	1.039-14	
1	2.437-9	1.357-10	5.673-10	1.032-10	7.035-11	0.557-11	0.343-12	3.451-11	4.029-13	
2	8.006-9	1.259-9	0.143-10	0.000-11	0.037-13	5.503-11	2.004-10	1.307-10	3.147-11	
3	3.560-5	3.332-9	2.137-9	1.291-10	1.195-10	1.125-10	1.420-13	7.944-12	1.620-13	
4	3.430-4	9.062-5	7.040-9	2.910-9	1.511-9	9.333-10	7.330-10	1.061-11	4.403-12	
5	1.133-2	7.203-4	2.040-5	2.147-7	2.620-11	2.523-9	3.792-12	3.919-9	1.011-9	
5	1.136-1	1.960-2	1.307-3	4.442-5	3.849-7	0.441-12	7.240-13	9.501-12	2.432-13	
7	2.720-1	1.473-1	2.800-2	2.414-3	9.621-5	9.392-7	7.547-10	6.063-12	5.633-9	
9	2.757-2	2.574-1	1.805-1	4.159-2	3.945-3	1.532-4	1.966-5	1.495-8	4.266-3	
9	1.271-1	4.009-3	2.205-1	2.114-1	3.731-2	6.154-3	2.722-4	4.263-6	4.543-3	
10	5.410-4	1.311-1	1.100-3	1.037-1	2.370-1	7.530-2	9.297-3	4.590-4	7.346-0	
11	6.342-2	1.297-2	1.155-1	1.454-2	1.457-1	2.554-1	9.720-2	1.342-2	7.159-4	
12	7.529-2	3.450-2	3.527-2	0.950-2	3.026-2	1.019-1	2.059-1	1.207-1	1.065-2	
13	1.031-2	7.751-2	1.200-2	5.903-2	5.911-2	6.577-2	6.291-2	2.600-1	1.453-1	
14	1.214-3	3.050-2	5.705-2	9.790-4	7.734-2	3.116-2	9.074-2	3.226-2	2.624-1	
15	2.620-2	1.321-3	5.206-2	4.943-2	1.953-3	0.593-2	1.079-2	1.091-1	1.223-2	
15	5.200-2	1.037-2	1.007-2	6.034-2	2.932-2	1.263-2	0.332-2	0.633-4	1.146-1	
17	5.924-2	3.015-2	1.407-3	2.347-2	3.969-2	1.227-2	2.057-2	7.162-2	1.850-3	
19	5.144-2	5.103-2	2.039-2	5.630-4	3.691-2	3.091-2	2.070-3	4.450-2	5.301-2	

Table 55
K_R FRANCK-CONDON FACTORS FOR Cu RED (3/2)

V	VV	0	1	2	3	4	5	6	7	8	9									
0	4.922-	1	3.715-	1	1.155-	1	1.911-	2	1.607-	3	5.739-	3	9.733-	7	3.692-	7	1.520-	4	2.726-	3
1	3.207-	1	4.357-	2	3.403-	1	2.219-	1	5.313-	2	5.272-	3	3.297-	4	1.074-	5	1.325-	6	1.919-	9
2	1.256-	1	2.431-	1	1.152-	2	2.139-	1	2.032-	1	1.025-	1	1.530-	2	1.140-	3	4.256-	5	2.103-	6
3	3.060-	2	1.950-	1	1.035-	2	0.705-	2	5.437-	2	2.390-	1	1.555-	1	3.124-	2	2.770-	3	1.190-	4
4	1.103-	2	9.453-	2	1.040-	1	1.506-	2	1.473-	1	1.051-	2	2.550-	1	2.055-	1	5.205-	2	5.654-	3
5	2.915-	3	3.527-	2	1.340-	1	1.259-	1	1.333-	3	1.593-	1	4.310-	4	2.033-	1	2.437-	1	7.015-	2
6	7.004-	4	1.154-	2	6.601-	2	1.432-	1	5.214-	2	2.013-	2	1.290-	1	2.175-	2	1.430-	1	2.671-	1
7	1.340-	4	3.599-	3	2.701-	2	9.430-	2	1.242-	1	1.725-	2	0.550-	2	0.370-	2	5.900-	2	0.219-	2
8	4.556-	5	1.052-	3	9.770-	3	4.707-	2	1.033-	1	3.035-	2	2.794-	4	9.512-	2	3.902-	2	9.650-	2
9	9.507-	6	2.950-	4	3.300-	3	1.994-	2	5.735-	2	1.134-	1	5.617-	2	7.151-	3	1.043-	1	1.037-	2
10	1.772-	6	7.531-	5	1.065-	3	7.059-	3	3.354-	2	9.292-	2	9.455-	2	1.955-	2	2.707-	2	9.430-	2
11	3.250-	7	1.025-	5	3.220-	4	2.777-	3	1.467-	2	4.052-	2	9.017-	2	7.059-	2	2.059-	3	5.137-	2
12	7.021-	8	4.210-	6	9.001-	5	9.540-	4	5.943-	3	2.414-	2	0.205-	2	0.770-	2	4.419-	2	0.277-	4
13	3.229-	8	1.035-	6	2.396-	5	3.009-	4	2.243-	3	1.101-	2	3.517-	2	7.172-	2	7.054-	2	2.114-	2
14	1.096-	8	3.034-	7	6.221-	6	9.269-	5	0.002-	4	4.499-	3	1.753-	2	4.636-	2	7.564-	2	5.924-	2
15	1.034-	8	1.039-	7	1.720-	6	2.593-	5	2.731-	4	1.757-	3	7.902-	3	2.573-	2	5.600-	2	7.201-	2
16	3.723-	9	4.412-	8	5.200-	7	7.054-	6	9.536-	5	5.560-	4	3.454-	3	1.296-	2	3.479-	2	6.255-	2
17	4.507-	10	1.532-	8	1.700-	7	1.905-	6	2.450-	5	2.279-	4	1.371-	3	5.946-	3	1.906-	2	4.343-	2
18	6.949-	11	3.534-	9	4.907-	8	5.910-	7	5.711-	6	7.235-	5	5.219-	4	2.596-	3	9.559-	3	2.615-	2

Table 55 (cont'd)

(CV RED (3/2))

V	VV	10	11	12	13	14	15	15	17	18
0	9.057-10	3.406-9	3.915-10	1.005-9	1.209-11	0.043-10	2.431-11	3.435-10	2.032-10	
1	1.145-7	1.753-3	1.346-9	7.645-9	9.657-11	2.019-9	1.176-11	1.128-9	1.653-11	
2	7.130-9	0.442-3	5.335-9	2.411-9	2.499-8	2.363-9	3.192-3	1.924-9	1.640-10	
3	4.592-6	2.103-9	0.071-8	6.016-8	1.451-13	2.534-8	1.000-9	0.691-10	5.720-9	
4	2.069-4	9.517-5	2.012-8	0.479-8	0.331-9	1.127-11	2.550-9	1.600-8	2.070-10	
5	1.017-2	5.924-4	1.072-5	7.025-8	7.198-8	7.051-8	4.170-11	3.605-8	2.644-8	
6	1.002-1	1.063-2	1.103-3	3.602-5	2.373-7	5.464-8	4.251-9	2.439-10	2.400-8	
7	2.736-1	1.400-1	2.531-2	1.925-3	0.545-3	3.920-7	5.100-9	4.601-8	2.053-10	
8	3.614-2	2.637-1	1.713-1	3.640-2	3.119-3	1.115-4	0.490-7	1.415-8	6.013-8	
9	1.212-1	3.740-3	2.444-1	2.022-1	5.000-2	4.791-3	1.930-4	1.010-5	1.556-9	
10	3.442-5	1.292-1	6.513-7	2.072-1	2.205-1	0.511-2	7.120-3	3.467-4	3.194-0	
11	7.171-2	6.699-3	1.209-1	7.047-3	1.679-1	2.492-1	0.449-2	1.010-2	4.607-4	
12	6.003-2	4.474-2	2.455-2	1.005-1	2.513-2	1.250-1	2.639-1	1.049-1	1.402-2	
13	1.026-2	7.596-2	2.005-2	4.650-2	7.307-2	4.915-2	0.797-2	2.716-1	1.266-1	
14	5.071-3	2.570-2	7.109-2	5.291-3	6.627-2	4.553-2	7.350-2	5.401-2	2.731-1	
15	3.956-2	7.075-5	4.102-2	5.032-2	2.360-5	7.952-2	2.319-2	9.409-2	2.975-2	
16	6.396-2	2.152-2	3.071-3	5.372-2	4.150-2	4.254-3	0.399-2	7.327-3	1.066-1	
17	6.441-2	5.950-2	0.009-3	1.241-2	5.000-2	2.390-2	1.537-2	7.960-2	3.360-4	
18	5.029-2	5.123-2	3.492-2	9.372-4	2.471-2	5.535-2	9.535-2	2.962-2	5.010-2	

Table 56

RKR FRANK-CONDON FACTORS FOR (Cv VIC.ET)

V	VV	0	1	2	3	4	5	7	8	9										
0	9.202-	1	7.301-	2	5.536-	3	3.020-	4	2.634-	5	1.116-	5	2.520-	9	7.579-	0	1.170-11	3.403-	4	
1	7.958-	2	7.911-	1	1.246-	1	1.434-	2	1.237-	3	9.552-	5	5.456-	5	2.514-	7	4.200-	3	3.962-10	
2	1.172-	3	1.424-	1	6.753-	1	1.543-	1	2.393-	2	2.670-	3	2.327-	4	1.534-	5	1.019-	0	6.002-	7
3	1.263-	0	2.050-	3	1.904-	1	5.941-	1	1.739-	1	3.332-	2	4.555-	3	5.417-	4	5.309-	5	7.050-	6
4	8.316-	7	2.597-	5	4.115-	3	2.313-	1	5.291-	1	1.023-	1	4.492-	2	7.036-	3	1.049-	3	1.402-	4
5	1.055-	7	1.749-	6	7.727-	5	5.304-	3	2.662-	1	4.035-	1	1.779-	1	5.526-	2	9.804-	3	1.710-	3
6	1.244-	7	1.233-	7	3.906-	0	2.430-	4	4.976-	2	2.320-	1	4.599-	1	1.630-	1	6.403-	2	1.236-	2
7	8.243-	9	0.040-	9	8.320-	0	1.071-	5	5.933-	4	3.156-	3	3.596-	1	4.559-	1	1.422-	1	7.061-	2
8	7.079-	0	2.507-	8	2.514-	7	3.739-	7	4.173-	5	1.619-	3	0.317-	4	3.122-	1	4.754-	1	1.146-	1
9	1.358-	8	2.763-	8	4.349-	8	3.052-	7	3.450-	6	4.435-	5	3.151-	3	1.550-	4	2.953-	1	5.190-	1
10	5.341-	9	1.850-	7	1.227-	9	4.041-	7	7.247-	9	1.523-	5	1.025-	5	5.010-	3	5.041-	3	2.532-	1
11	1.047-	9	2.359-	0	2.399-	9	2.390-	0	4.639-	7	1.971-	0	4.111-	5	2.174-	5	6.664-	3	2.040-	2
12	6.857-10	10	6.352-	9	3.511-	8	3.943-	9	1.335-	7	2.514-	5	5.592-	7	6.627-	5	3.395-	4	6.380-	3
13	1.522-	9	2.354-	0	7.370-10	10	1.102-10	10	2.073-	0	1.100-	7	1.957-	7	3.535-	6	7.617-	5	1.434-	3
14	1.915-	9	1.239-	0	2.550-	0	3.205-11	11	1.040-	7	3.979-	9	2.924-	9	4.146-	7	1.632-	5	2.239-	5
15	8.215-11	11	3.152-10	10	5.003-	0	1.452-	0	4.653-	0	2.295-	7	1.395-	9	3.070-	7	5.003-	7	5.109-	5
16	6.715-10	10	1.354-	9	2.629-	0	5.354-	0	1.910-	0	2.335-	7	1.097-	7	1.642-	7	1.247-	6	6.005-	7
17	1.443-	9	1.315-	9	2.063-	9	5.754-	0	3.020-	0	1.142-	7	2.931-	7	2.090-	7	2.009-	7	2.403-	6
18	7.204-10	10	4.456-11	11	9.781-10	10	2.303-	0	4.994-	0	1.037-	0	3.059-	7	2.341-	7	1.467-	7	1.297-	6

Table 56 (cont'd)

(CM VIO-ET)

V	VV	10	11	12	13	14	15	16	17	18
0	2.075-	9	5.363-	9	2.151-10	6.209-11	1.030-10	3.534-11	9.761-13	1.965- 9
1	7.051-	8	1.055-	7	9.603- 8	6.497- 9	5.969- 9	1.310- 8	7.634- 9	3.409- 9
2	2.453-	7	1.037-	7	2.225- 7	1.550- 7	2.154- 9	1.471- 8	5.930- 9	6.295- 8
3	2.651-	6	1.336-	6	5.074- 7	1.049- 7	5.331- 8	1.531- 9	3.935- 9	1.320- 7
4	2.604-	5	5.099-	5	2.627- 6	7.979- 7	9.507- 9	1.555-10	3.741- 8	1.161- 7
5	2.763-	4	4.448-	5	9.053- 6	3.029- 6	0.069- 7	1.401- 8	1.055- 7	1.958- 7
6	2.430-	3	4.266-	4	7.410- 5	1.184- 5	2.227- 5	4.937- 7	5.593-10	3.072- 7
7	1.405-	2	3.132-	3	5.511- 4	9.034- 5	1.541- 5	1.623- 6	5.517- 9	3.363- 9
8	7.637-	2	1.443-	2	3.716- 3	6.590- 4	1.130- 4	1.511- 5	1.570- 5	2.447- 9
9	0.140-	2	0.254-	2	1.342- 2	4.122- 3	7.110- 4	1.315- 4	1.695- 5	1.211- 6
10	5.011-	1	4.915-	2	9.001- 2	1.107- 2	4.537- 3	7.030- 4	1.416- 4	1.917- 3
11	1.090-	1	0.456-	1	2.231- 2	1.022- 1	7.776- 3	5.050- 3	6.593- 4	1.633- 4
12	4.020-	2	1.126-	1	6.974- 1	4.774- 3	1.134- 1	4.163- 3	5.942- 3	5.026- 4
13	3.656-	3	9.557-	2	4.234- 2	7.135- 1	0.695- 3	1.440- 1	9.056- 4	7.774- 3
14	3.350-	3	3.491-	4	1.202- 1	2.452- 3	6.766- 1	7.555- 3	1.779- 1	2.534- 4
15	3.050-	5	5.460-	3	2.219- 3	1.375- 1	1.626- 2	5.709- 1	2.127- 2	2.166- 1
16	7.401-	5	5.115-	4	5.615- 3	1.613- 2	1.229- 1	9.263- 2	4.316- 1	3.206- 2
17	1.244-	5	4.596-	5	1.933- 3	2.921- 3	4.471- 2	7.534- 2	2.105- 1	2.690- 1
18	6.677-	7	5.041-	5	6.002- 6	3.995- 3	5.601- 5	7.076- 2	2.233- 2	3.233- 1
19										

Table 57

RKR FRANK-CONDON FACTORS FOR CO (FM 4)

v	u	1	2	3	4	5	6	7	8	9	10	11	12
1	1.111-1	2.000-1	2.905-1	1.390-1	3.704-2	3.415-2	9.172-3	2.337-3	3.939-4	5.474-5	7.790-6	9.090-7	3.201-3
2	2.100-1	1.553-1	2.352-1	7.799-2	1.979-1	1.059-1	1.040-1	4.355-2	1.210-2	2.305-3	5.395-4	9.137-5	1.231-5
3	2.370-1	1.134-2	9.147-2	1.123-1	3.350-3	0.524-2	1.717-1	1.561-1	9.233-2	3.651-2	1.000-2	2.502-3	3.102-4
4	1.843-1	2.357-2	1.150-1	1.013-4	9.433-2	7.740-2	1.763-3	7.351-2	1.653-1	1.434-1	7.519-2	2.910-2	9.453-3
5	1.174-1	9.359-2	3.029-2	6.210-2	5.057-2	1.051-2	1.021-1	4.254-2	6.984-3	1.330-1	1.505-1	1.211-1	5.044-2
6	0.620-2	1.243-1	1.243-3	9.022-2	3.026-4	0.556-2	1.570-2	4.135-2	9.345-2	1.340-2	2.776-2	1.210-1	1.470-1
7	3.443-2	1.102-1	3.334-2	3.554-2	4.947-2	3.440-2	3.013-2	6.749-2	1.215-4	7.400-2	6.400-2	2.050-4	5.640-2
8	1.607-2	9.725-2	9.273-2	5.700-4	7.353-2	1.422-3	6.964-2	3.213-4	6.575-2	2.717-2	1.950-2	3.624-2	2.947-2
9	7.805-3	5.572-2	9.756-2	1.519-2	3.722-2	4.174-2	2.071-2	4.077-2	3.246-2	1.961-2	0.633-2	1.299-3	5.311-2
10	3.552-3	3.190-2	8.555-2	5.144-2	3.219-3	5.147-2	2.104-3	5.561-2	2.354-3	5.999-2	9.029-4	5.523-2	5.303-2
11	1.531-3	1.730-2	6.420-2	7.456-2	5.049-3	3.613-2	3.392-2	1.425-2	4.240-2	1.349-2	3.747-2	3.130-2	1.300-2
12	6.563-4	9.993-3	4.319-2	7.783-2	3.140-2	6.434-3	5.203-2	1.701-3	4.537-2	5.306-3	4.529-2	3.101-3	5.440-2
13	2.710-4	4.471-3	2.550-2	6.603-2	5.520-2	1.393-3	3.513-2	2.541-2	1.134-2	4.805-2	4.765-3	4.215-2	9.855-3
14	1.167-4	2.100-3	1.557-2	4.304-2	6.000-2	1.001-2	9.074-3	4.363-2	1.011-3	3.035-2	9.659-3	3.313-2	1.021-2
15	4.314-5	1.029-3	1.332-3	3.334-2	6.200-2	3.957-2	1.009-3	3.420-2	1.950-2	1.067-2	3.652-2	2.015-3	4.017-2
16	1.035-5	4.700-4	4.549-3	2.155-2	5.103-2	5.375-2	0.912-3	1.303-2	3.573-2	2.640-4	3.397-2	3.700-3	2.541-2
17	6.002-6	2.003-4	2.310-3	1.294-2	3.050-2	3.674-2	2.613-2	0.579-4	3.229-2	1.296-2	1.149-2	3.145-2	1.399-3
18	2.272-6	0.915-5	1.146-3	7.476-3	2.670-2	5.147-2	4.119-2	2.071-3	1.610-2	2.752-2	3.794-3	3.110-2	7.256-3
19	5.597-7	3.615-5	5.470-4	4.154-3	1.750-2	4.197-2	4.069-2	1.358-2	3.561-3	2.912-2	6.604-3	1.393-2	2.491-2
20	3.251-7	1.340-5	2.493-4	2.234-3	1.090-2	3.146-2	4.023-2	2.705-2	1.554-4	1.927-2	1.054-2	1.265-3	2.019-2
21	1.152-7	4.333-6	1.056-4	1.125-3	6.410-3	2.155-2	4.110-2	3.356-2	5.233-3	7.390-3	2.270-2	1.569-3	1.602-2

Table 57 (cont'd)

(CO 474. +)

V	13	14	15	16	17	18	19	20	21	22	23	24
0	0.041- 8	2.942- 3	1.339- 4	3.053-10	1.425- 9	1.053- 9	1.175-10	3.411-11	1.214-13	5.537-12	3.636-12	1.221-13
1	2.096- 6	3.797- 7	3.562- 9	4.642- 8	2.534- 3	1.130- 8	3.091- 9	3.596-10	3.093-13	2.031- 9	5.242- 9	1.750-14
2	3.685- 5	1.514- 5	1.032- 6	0.523-14	1.207- 8	3.429- 8	5.712- 9	2.447- 8	1.565- 8	1.507- 8	1.097-11	4.790-13
3	2.162- 3	4.206- 4	0.231- 5	3.944- 6	2.250- 7	3.004- 7	1.040- 7	3.759-10	7.912- 8	1.127-11	5.376- 4	9.719- 3
4	2.298- 2	6.476- 3	1.372- 3	2.250- 4	3.012- 5	5.551- 6	1.007- 6	7.953- 8	1.079- 7	1.424- 4	3.430- 4	2.430- 8
5	1.006- 1	4.633- 2	1.555- 2	3.994- 3	0.301- 4	1.555- 4	2.723- 5	3.959- 6	3.333- 8	1.324- 7	2.549- 9	1.352- 7
6	1.362- 1	1.322- 1	7.040- 2	3.265- 2	1.431- 2	2.026- 3	5.467- 4	0.033- 5	9.423- 6	2.009- 7	4.620- 8	3.395- 7
7	7.496- 3	0.036- 2	1.442- 1	1.121- 1	3.095- 2	2.274- 2	3.574- 3	1.430- 3	2.634- 4	3.720- 5	4.039- 6	1.070- 5
8	7.177- 2	3.233- 3	3.216- 2	1.141- 1	1.333- 1	9.122- 2	4.230- 2	1.430- 2	3.022- 3	0.201- 4	1.402- 4	2.411- 5
9	9.900- 3	7.634- 2	4.147- 2	9.430- 4	3.409- 2	1.332- 1	1.205- 1	3.959- 2	2.902- 2	9.224- 3	2.254- 3	4.335- 4
10	6.209- 2	4.521- 3	3.044- 2	7.322- 2	1.352- 2	1.635- 2	9.599- 2	1.325- 1	1.009- 1	5.144- 2	1.944- 2	5.390- 3
11	1.910- 3	4.530- 2	3.701- 2	3.193- 3	6.457- 2	5.050- 2	2.505- 4	4.539- 2	1.103- 1	1.242- 1	7.923- 2	3.592- 2
12	3.303- 2	3.442- 2	3.114- 3	3.014- 2	0.911- 3	2.577- 2	7.145- 2	2.226- 2	7.026- 3	7.075- 2	1.300- 1	1.114- 1
13	3.949- 2	2.901- 3	3.036- 2	3.244- 3	3.710- 2	4.150- 2	4.110- 4	3.341- 2	5.762- 2	3.236- 3	3.125- 2	1.195- 1
14	1.925- 3	3.905- 2	0.245- 3	2.995- 2	3.114- 2	5.090- 3	3.407- 2	1.425- 2	1.624- 2	6.064- 2	3.006- 2	2.024- 3
15	1.460- 2	2.502- 2	1.193- 2	3.576- 2	2.144- 3	4.590- 2	3.363- 3	2.927- 2	4.455- 2	1.776- 4	4.317- 2	6.440- 2
16	3.547- 2	1.644- 4	3.737- 2	1.005- 3	3.674- 2	0.900- 3	2.424- 2	3.279- 2	1.910- 3	4.070- 2	2.552- 2	9.376- 3
17	2.130- 2	1.481- 2	1.705- 2	1.632- 2	2.206- 2	9.930- 3	3.374- 2	7.121- 4	4.140- 2	9.409- 3	1.993- 2	4.590- 2
18	1.092- 3	3.033- 2	1.910- 5	3.220- 2	1.412- 5	3.371- 2	1.454- 3	3.121- 2	1.203- 2	1.663- 2	3.502- 2	4.959- 3
19	3.751- 3	2.012- 2	1.156- 2	1.490- 2	1.513- 2	1.501- 2	1.331- 2	2.240- 2	5.577- 3	3.350- 2	7.435- 5	3.392- 2
20	1.616- 2	3.041- 3	2.352- 2	3.470- 4	2.596- 2	2.239- 5	2.731- 2	3.702- 4	2.722- 2	4.309- 3	2.134- 2	1.791- 2

RR2 FRANCK-CONDON FACTORS FOR (N2) 151.4

Table 58

V	V'	0	1	2	3	4	5	6
0	4.003-1	3.304-1	1.662-1	6.603-2	2.304-2	7.960-3	2.577-3	
1	3.990-1	2.903-3	1.503-1	1.963-1	1.303-1	5.555-2	2.038-2	
2	1.010-1	2.743-1	6.060-2	2.203-2	1.245-1	1.427-1	1.009-1	
3	3.411-2	2.767-1	9.595-2	1.515-1	3.131-3	4.233-2	1.077-1	
4	4.010-3	9.592-2	2.973-1	7.555-3	1.510-1	5.114-2	2.211-3	
5	2.665-4	1.024-2	1.600-1	2.431-1	1.046-2	9.520-2	9.404-2	
6	1.000-5	1.424-3	3.093-2	2.295-1	1.553-1	5.903-2	3.534-2	
7	2.527-7	6.530-5	4.337-3	7.163-2	2.655-1	7.447-2	1.056-1	
8	3.912-9	1.398-6	2.337-4	9.002-3	1.113-1	2.712-1	2.005-2	
9	2.559-10	3.574-11	5.539-6	6.303-4	1.099-2	1.554-1	2.487-1	
10	3.150-9	1.243-12	1.357-4	1.660-5	1.420-3	3.235-2	1.975-1	
11	3.231-10	2.490-9	3.377-12	0.925-5	4.230-5	2.029-3	5.036-2	
12	4.427-10	1.335-9	2.924-3	9.562-10	3.510-7	9.730-5	5.100-3	
13	5.016-10	7.532-11	6.955-10	2.020-9	3.225-9	0.540-7	1.966-4	
14	4.000-12	0.431-10	1.181-10	1.205-9	7.420-11	2.500-3	1.014-6	
15	1.209-10	3.304-10	6.717-10	4.307-10	1.503-9	2.621-10	4.156-9	
16	7.521-11	1.026-11	5.034-10	1.400-9	5.541-13	3.090-10	5.698-10	
17	1.011-14	2.320-10	4.560-11	3.595-10	1.507-9	1.312-10	2.796-10	

Table 58 (cont'd)

(V(2) 1ST.4)

V	VV	7	8	9	10	11	12	13						
1	0.221-	4	2.611-	4	0.295-	3	2.645-	3	0.524-	3	2.011-	3	9.655-	7
2	1.127-	2	4.262-	3	1.572-	3	5.745-	4	2.091-	4	7.602-	3	2.770-	5
3	5.617-	2	2.722-	2	1.214-	2	5.153-	3	2.130-	3	0.665-	4	3.439-	4
4	1.114-	1	0.006-	2	4.727-	2	2.402-	2	1.209-	2	5.513-	3	2.532-	3
5	5.409-	2	9.391-	2	0.975-	2	6.509-	2	4.017-	2	2.239-	2	1.100-	2
6	9.739-	3	1.404-	2	5.955-	2	0.133-	2	7.392-	2	5.390-	2	3.450-	2
7	1.043-	1	3.335-	2	5.372-	1	2.511-	2	5.933-	2	7.310-	2	5.154-	2
8	3.054-	3	0.142-	2	6.755-	2	1.064-	2	3.095-	3	3.170-	2	5.497-	2
9	1.280-	1	4.732-	3	4.454-	2	7.713-	2	3.312-	2	1.012-	3	9.068-	3
10	1.309-	4	1.199-	1	2.917-	2	1.356-	2	5.595-	2	5.200-	2	1.292-	2
11	2.054-	1	1.022-	2	0.952-	2	5.092-	2	2.610-	4	4.200-	2	5.956-	2
12	2.334-	1	1.514-	1	3.075-	2	5.163-	2	7.911-	2	6.000-	3	1.758-	2
13	7.292-	2	2.591-	1	9.664-	2	7.263-	2	1.961-	2	0.245-	2	2.413-	2
14	0.519-	3	9.340-	2	2.722-	1	5.003-	2	1.002-	1	2.209-	3	6.930-	2
15	3.665-	4	1.341-	2	1.294-	1	2.712-	1	1.757-	2	1.142-	1	1.913-	3
16	3.597-	6	6.307-	4	2.000-	2	1.611-	1	2.570-	1	1.750-	3	1.121-	1
17	3.126-	9	0.543-	6	1.050-	3	2.073-	2	1.933-	1	2.316-	1	1.996-	3
18	1.417-	9	3.135-12	12	1.055-	5	1.622-	3	3.950-	2	2.250-	1	1.907-	1

Table 59

RKR FRANCK-CONDON FACTORS FOR (V(2) 2VJ,+))

VV	0	1	2	3	4	5	6	7	8	
V	0	4.524- 1	3.272- 1	1.453- 1	5.162- 2	1.606- 2	4.522- 3	1.256- 3	3.348- 4	9.630- 5
	1	3.925- 1	2.177- 2	2.036- 1	1.983- 1	1.134- 1	4.712- 2	1.729- 2	5.769- 3	1.849- 3
	2	1.331- 1	3.415- 1	2.420- 2	6.317- 2	1.634- 1	1.307- 1	7.929- 2	3.632- 2	1.454- 2
	3	2.043- 2	2.530- 1	2.102- 1	0.923- 2	4.734- 3	9.316- 2	1.303- 2	9.865- 2	5.550- 2
	4	9.693- 4	5.384- 2	3.307- 1	1.199- 1	1.131- 1	3.915- 3	4.031- 2	1.001- 1	1.001- 1

VV	9	10	11	12	13	14	15	16	17	
V	0	2.180- 5	5.433- 5	1.354- 5	3.454- 7	3.229- 9	2.530- 8	7.954- 9	2.407- 9	7.397- 10
	1	5.436- 4	1.584- 4	4.512- 5	1.268- 5	3.563- 6	1.023- 6	3.033- 7	9.163- 8	2.642- 8
	2	5.320- 3	1.036- 3	6.070- 4	1.951- 4	0.130- 5	1.833- 5	5.755- 5	1.740- 6	5.121- 7
	3	2.620- 2	1.111- 2	4.544- 3	1.606- 3	3.739- 4	1.975- 4	5.656- 5	2.369- 5	6.740- 6
	4	6.802- 2	3.736- 2	1.735- 2	7.070- 3	3.217- 3	1.240- 3	4.650- 4	1.607- 4	5.903- 5

Table 60

RKR FRANCK-CONDON FACTORS FJR(V2 B-M 1)

V	0	1	2	3	4	5	6	7	8	9	10
0	2.753-7	3.797-6	2.719-5	2.719-5	5.022-4	1.540-3	3.909-3	0.925-3	1.756-2	3.083-2	4.050-2
1	3.751-6	4.532-5	2.022-4	2.022-4	3.013-3	9.030-3	2.005-2	3.736-2	5.703-2	7.440-2	0.209-2
2	2.592-5	2.723-4	1.461-3	1.461-3	1.404-2	2.939-2	4.344-2	6.033-2	7.223-2	5.937-2	3.205-2
3	1.212-4	1.497-3	2.012-3	5.012-3	3.203-2	5.400-2	6.741-2	6.131-2	3.650-2	9.133-3	4.161-4
4	4.314-4	3.331-3	1.277-2	1.277-2	5.304-2	6.533-2	5.330-2	2.351-2	1.402-3	7.062-3	3.115-2
5	1.247-3	0.100-3	2.502-2	2.502-2	6.303-2	5.074-2	1.090-2	1.237-4	1.291-2	3.649-2	3.027-2
6	3.449-3	1.645-2	4.109-2	4.109-2	5.373-2	2.064-2	9.046-2	1.433-2	3.009-2	3.006-2	5.350-3
7	6.493-3	2.055-2	5.074-2	5.074-2	2.047-2	9.719-4	1.210-2	3.550-2	2.760-2	3.176-3	6.012-3
8	1.220-2	4.306-2	6.390-2	6.390-2	5.630-2	6.534-3	1.239-2	2.911-2	3.606-3	6.033-3	2.000-2
9	2.090-2	5.600-2	5.909-2	5.909-2	0.009-2	2.591-2	3.292-2	5.723-3	4.519-3	2.709-2	2.102-2
10	3.279-2	0.606-2	4.312-2	4.312-2	1.402-2	3.553-2	1.333-2	1.192-3	2.346-2	2.290-2	1.242-3
11	4.729-2	6.725-2	2.222-2	2.222-2	3.053-2	2.524-2	2.990-4	1.662-2	2.610-2	3.632-3	7.752-3
12	6.331-2	5.009-2	5.402-3	5.402-3	3.456-3	7.100-3	6.074-3	2.746-2	9.322-3	3.103-3	2.332-2
13	7.900-2	4.273-2	5.620-3	5.620-3	2.310-2	0.732-3	2.200-2	1.039-2	4.500-5	1.054-2	1.690-2
14	9.239-2	2.355-2	7.135-3	7.135-3	7.063-3	9.040-3	2.595-2	3.152-3	1.005-2	2.160-2	1.750-3
15	1.017-1	7.493-3	2.150-2	2.150-2	5.962-0	2.231-2	1.460-2	1.547-3	2.160-2	0.109-3	3.026-3
16	1.047-1	1.142-4	3.454-2	3.454-2	6.511-3	2.537-2	1.917-3	1.330-2	1.730-2	1.607-5	1.673-2
17	1.003-1	4.477-3	3.021-2	3.021-2	1.907-2	1.550-2	1.032-3	2.135-2	4.219-3	0.262-3	1.726-2
18	0.919-2	1.915-2	3.064-2	3.064-2	2.567-2	3.350-3	1.232-2	1.579-2	5.010-4	1.000-2	5.366-3
19	7.193-2	3.759-2	1.644-2	1.644-2	2.055-2	3.512-4	1.956-2	4.186-3	0.853-3	1.452-2	1.392-4
20	1.534-2	1.766-2	7.272-4	7.272-4	2.100-3	2.975-3	4.351-3	2.050-4	5.102-3	6.166-4	2.900-3

Table 60 (cont'd)

RKR FRANCIS-CONJOY FACTORS - J2 (V2 3-M 1)

V	11	12	13	14	15	16	17	18	19	20	21
1	6.934-2	9.611-2	1.068-1	1.102-1	1.162-1	1.004-1	0.976-2	6.972-2	5.005-2	3.316-2	2.012-2
2	7.515-2	5.404-2	2.605-2	5.341-3	5.599-4	1.446-2	4.133-2	6.973-2	0.914-2	9.403-2	0.493-2
3	7.815-3	3.995-4	1.530-2	4.080-2	5.686-2	5.062-2	2.720-2	4.973-3	0.986-3	2.161-2	5.517-2
4	1.663-2	4.001-2	4.726-2	2.943-2	5.803-3	1.757-3	2.223-2	4.633-2	4.971-2	2.892-2	4.729-3
5	4.334-2	2.802-2	4.550-3	3.111-3	2.530-2	4.200-2	3.030-2	6.737-3	1.012-3	2.420-2	4.756-2
6	1.246-2	1.701-4	1.712-2	3.052-2	2.001-2	4.025-3	3.566-3	2.697-2	3.929-2	2.164-2	0.809-4
7	3.652-3	2.620-2	3.264-2	1.150-2	4.190-4	1.914-2	3.433-2	1.913-2	3.706-4	1.246-2	3.509-2
8	2.903-2	2.600-2	3.552-3	5.739-3	2.778-2	2.565-2	3.600-3	5.771-3	2.866-2	2.732-2	4.027-3
9	2.183-2	1.024-3	1.056-2	2.885-2	1.593-2	2.013-10	1.633-2	2.934-2	1.096-2	9.835-4	2.233-2
10	5.916-4	1.233-2	2.744-2	1.031-2	1.231-3	2.143-2	2.320-2	2.390-3	0.264-3	2.701-2	1.409-2
11	1.119-2	2.619-2	0.346-3	2.448-3	2.273-2	1.707-2	1.374-4	1.440-2	2.012-2	5.270-3	5.230-3
12	2.520-2	9.065-3	2.237-3	2.200-2	1.522-2	3.521-3	1.536-2	2.031-2	1.326-3	1.077-2	2.444-2
13	1.200-2	9.414-4	1.996-2	1.513-2	4.337-5	1.679-2	1.821-2	3.137-4	1.350-2	2.111-2	1.669-3
14	2.205-7	1.630-2	1.689-2	5.007-3	1.474-2	1.740-2	2.356-4	1.334-2	1.057-2	5.733-4	1.273-2
15	1.057-2	1.937-2	1.133-3	1.111-2	1.821-2	7.130-4	1.175-2	1.752-2	4.654-4	1.207-2	1.720-2
16	2.035-2	4.592-3	5.129-3	1.902-2	2.413-3	0.475-3	1.791-2	9.091-4	1.090-2	1.654-2	1.550-4
17	1.090-2	1.459-3	1.815-2	6.047-3	4.310-3	1.802-2	2.534-3	0.830-3	1.670-2	5.206-4	1.215-2
18	2.260-4	1.355-2	1.160-2	7.776-4	1.650-2	5.979-3	4.154-3	1.732-2	1.794-3	9.198-3	1.452-2
19	5.753-3	1.633-2	4.633-4	1.203-2	1.003-2	0.103-4	1.372-2	4.750-3	5.251-3	1.557-2	5.107-4
20	1.515-2	5.476-3	4.670-3	1.401-2	3.570-4	1.131-2	9.149-3	1.290-3	1.494-2	2.747-3	7.241-3
21	3.139-3	2.906-4	4.360-3	7.142-4	2.296-3	3.353-3	0.890-5	4.800-3	1.153-3	1.667-3	3.730-3

Table 61 RK2 FRANCK-CONDON FACTORS FOR N_2 B-M 21

v'	v''	0	1	2	3	4	5	5	7	8	9	10
1	1	1.155-2	3.500-2	6.620-2	6.620-2	1.176-1	1.200-1	1.261-1	1.136-1	9.436-2	7.296-2	5.260-2
1	1	4.793-2	1.023-1	1.193-1	1.193-1	5.403-2	1.611-2	1.351-4	9.526-3	3.562-2	6.469-2	0.534-2
2	1	1.011-1	1.311-1	7.001-2	7.001-2	3.025-3	3.347-2	3.369-2	6.554-2	4.002-2	1.172-2	1.251-5
3	1	1.436-1	9.025-2	5.462-3	5.462-3	6.021-2	6.033-2	2.372-2	2.530-4	1.420-2	4.531-2	5.970-2
4	1	1.590-1	2.943-2	1.530-2	1.530-2	4.733-2	4.350-3	1.051-2	4.496-2	5.029-2	2.125-2	2.079-4
5	1	1.506-1	3.666-4	5.409-2	6.409-2	1.605-3	2.221-2	5.220-2	2.997-2	7.097-4	1.532-2	4.446-2
6	1	1.233-1	1.425-2	0.004-2	0.004-2	2.062-2	5.250-2	1.914-2	1.436-3	3.220-2	4.222-2	1.250-2
7	1	9.122-2	4.074-2	5.222-2	5.222-2	5.379-2	2.245-2	2.471-3	3.654-2	3.327-2	2.070-3	1.360-2
8	1	6.204-2	7.050-2	1.507-2	1.507-2	4.151-2	6.078-3	3.415-2	3.159-2	5.173-4	2.030-2	3.695-2
9	1	4.070-2	9.103-2	1.109-4	1.109-4	9.240-3	2.119-2	3.033-2	1.020-3	1.000-2	3.405-2	5.255-3
10	1	2.550-2	0.757-2	0.320-3	0.320-3	1.003-3	4.260-2	1.116-2	1.030-2	3.431-2	6.533-3	0.045-3
11	1	1.573-2	7.477-2	2.793-2	2.793-2	1.940-2	3.444-2	4.300-4	3.221-2	1.409-2	4.137-3	2.941-2
12	1	9.629-3	5.923-2	4.644-2	4.644-2	4.007-2	1.206-2	1.574-2	2.046-2	3.559-7	2.433-2	1.683-2
13	1	5.067-3	4.426-2	5.710-2	5.710-2	4.730-2	1.597-4	3.172-2	0.973-3	1.132-2	2.539-2	3.901-4
14	1	3.619-3	3.200-2	5.960-2	5.960-2	3.976-2	5.990-3	3.105-2	2.547-5	2.562-2	0.056-3	7.530-3
15	1	2.253-3	2.270-2	5.509-2	5.509-2	2.445-2	2.092-2	1.753-2	7.602-3	2.416-2	1.011-6	2.110-2
16	1	1.424-3	1.500-2	4.003-2	4.003-2	1.040-2	3.357-2	4.534-3	2.029-2	1.153-2	6.601-3	2.100-2
17	1	9.126-4	1.103-2	4.053-2	4.053-2	2.201-3	3.795-2	9.502-6	2.620-2	1.462-3	1.744-2	9.754-3
18	1	5.977-4	7.700-3	3.266-2	3.266-2	1.310-5	3.445-2	4.357-3	2.230-2	9.030-4	2.096-2	9.015-4
19	1	3.965-4	5.376-3	2.561-2	2.561-2	2.114-3	2.614-2	1.310-2	1.406-2	7.670-3	1.571-2	1.255-3
20	1	2.672-4	3.775-3	1.974-2	1.974-2	0.150-3	1.695-2	2.125-2	5.555-3	1.527-2	7.319-3	7.410-3
21	1	1.759-4	2.569-3	1.443-2	1.443-2	9.769-3	0.023-3	2.474-2	0.124-4	1.037-2	1.433-3	1.247-2
22	1	9.437-5	1.411-3	0.356-3	0.356-3	9.016-3	3.240-3	1.064-2	3.104-5	1.329-2	7.765-9	1.032-2
23	1	4.023-5	7.424-4	4.657-3	4.657-3	0.255-3	5.045-4	1.313-2	1.306-3	0.095-3	1.179-3	6.794-3
24	1	3.100-5	5.007-4	3.260-3	3.260-3	7.093-3	3.632-3	1.016-2	2.006-3	5.100-3	2.755-3	4.244-3

Table 6f (cont'd)

v	v'	11	12	13	14	15	16	17	18	19	20	21												
1	3.547-	2	2.241-	2	1.323-	3	3.753-	3	1.741-	3	7.770-	4	3.133-	4	1.157-	4	3.931-	5	1.227-	5	3.434-	4	3.434-	4
1	3.130-	2	3.454-	2	5.933-	2	5.352-	2	1.906-	2	1.072-	2	5.245-	3	2.338-	3	9.402-	4	3.434-	4	3.434-	4	3.434-	4
2	1.256-	2	4.640-	2	6.042-	2	0.317-	2	6.026-	2	4.917-	2	3.103-	2	1.744-	2	8.720-	3	3.044-	3	3.044-	3	3.044-	3
3	4.249-	2	1.425-	2	3.231-	5	1.189-	2	0.997-	2	0.290-	2	7.740-	2	6.221-	2	3.945-	2	2.263-	2	2.263-	2	2.263-	2
4	1.414-	2	4.309-	2	5.324-	2	3.337-	2	1.541-	3	2.433-	2	5.044-	2	9.098-	2	0.293-	2	6.710-	2	6.710-	2	6.710-	2
5	4.002-	2	1.649-	2	1.335-	3	2.545-	2	4.999-	2	1.535-	2	4.713-	7	1.066-	2	5.307-	2	0.247-	2	0.247-	2	0.247-	2
6	1.559-	3	2.805-	2	4.355-	2	2.202-	2	3.749-	4	4.355-	2	4.651-	2	1.981-	2	1.525-	4	1.645-	2	1.645-	2	1.645-	2
7	3.931-	2	2.445-	2	4.797-	4	1.532-	2	4.004-	2	2.593-	3	0.740-	3	3.308-	2	4.653-	2	1.354-	2	1.354-	2	1.354-	2
8	9.723-	3	3.764-	3	3.120-	2	3.041-	2	3.575-	3	3.581-	2	3.154-	2	4.368-	3	7.133-	3	3.057-	2	3.057-	2	3.057-	2
9	9.273-	3	3.355-	2	1.650-	2	4.345-	4	2.350-	2	5.537-	3	5.141-	3	3.254-	2	3.134-	2	4.001-	2	4.001-	2	4.001-	2
10	3.200-	2	1.067-	2	3.296-	3	2.820-	2	2.050-	2	1.058-	2	3.150-	2	0.198-	3	4.017-	3	3.136-	2	3.136-	2	3.136-	2
11	1.141-	2	3.520-	3	2.748-	2	1.457-	2	0.253-	4	2.231-	2	4.903-	4	1.539-	2	3.053-	2	7.971-	3	7.971-	3	7.971-	3
12	1.005-	3	2.472-	2	1.475-	2	1.003-	3	2.309-	2	1.822-	4	2.025-	2	2.272-	2	0.691-	4	1.436-	2	1.436-	2	1.436-	2
13	1.794-	2	1.085-	2	5.591-	5	1.397-	2	1.650-	2	1.977-	2	1.039-	2	1.189-	6	1.002-	2	2.180-	2	2.180-	2	2.180-	2
14	2.312-	2	1.560-	3	1.340-	2	1.951-	2	1.152-	4	1.751-	2	3.599-	6	1.732-	2	1.010-	2	2.289-	5	2.289-	5	2.289-	5
15	9.350-	3	4.478-	3	2.164-	2	2.430-	3	1.016-	2	5.093-	4	1.350-	2	1.777-	2	7.222-	5	1.580-	2	1.580-	2	1.580-	2
16	6.521-	3	1.710-	2	1.051-	2	2.624-	3	1.999-	2	7.534-	3	1.002-	2	1.056-	3	1.232-	2	1.703-	2	1.703-	2	1.703-	2
17	5.417-	3	1.045-	2	3.751-	4	1.424-	2	1.125-	2	1.004-	2	4.755-	3	6.060-	3	1.021-	2	1.192-	3	1.192-	3	1.192-	3
18	1.534-	2	0.068-	3	3.738-	3	1.717-	2	0.312-	4	1.143-	2	0.355-	4	1.668-	2	5.205-	3	5.360-	3	5.360-	3	5.360-	3
19	1.034-	2	0.582-	4	1.256-	2	0.972-	3	2.499-	3	1.209-	2	1.019-	2	1.154-	2	4.736-	4	1.562-	2	1.562-	2	1.562-	2
20	1.317-	2	1.215-	3	1.561-	2	1.152-	3	1.032-	2	1.720-	3	1.475-	2	1.654-	3	0.602-	3	1.136-	2	1.136-	2	1.136-	2
21	5.470-	3	6.426-	3	1.005-	2	6.449-	4	1.305-	2	0.201-	3	0.907-	3	9.133-	4	1.297-	2	2.014-	3	2.014-	3	2.014-	3
22	9.571-	4	7.715-	3	4.019-	3	3.037-	3	7.016-	3	0.458-	3	2.113-	3	4.053-	3	7.149-	3	1.090-	4	1.090-	4	1.090-	4
23	1.146-	4	6.916-	4	3.170-	4	5.255-	3	2.423-	3	5.337-	3	5.297-	3	5.006-	3	1.279-	3	3.024-	3	3.024-	3	3.024-	3
24	1.148-	3	5.210-	3	1.166-	4	5.298-	3	3.600-	4	2.431-	3	1.374-	3	4.595-	3	0.407-	7	4.505-	3	4.505-	3	4.505-	3

Table 62

RK2 FRANCK-CONDON FACTORS FJR(N2+ MEINEL)

v	v'	0	1	2	3	4	5	6	7	8	9	10
1	5	1.106-1	3.646-1	1.062-1	1.652-2	1.497-3	7.010-3	2.293-6	1.923-9	2.033-10	1.390-11	3.490-11
1	1	3.160-1	5.256-2	3.531-1	2.177-1	5.306-2	6.560-3	4.344-4	1.439-5	1.548-7	3.046-11	2.617-10
2	1	1.239-1	2.454-1	1.034-2	2.156-1	2.049-1	1.042-1	1.760-2	1.307-3	5.305-5	6.712-7	1.401-10
3	3	3.753-2	1.920-1	1.129-1	0.003-2	0.504-2	2.953-1	1.604-1	3.407-2	3.349-3	1.469-4	2.066-6
4	4	1.054-2	3.196-2	1.017-1	1.552-2	1.515-1	1.316-2	2.595-1	2.110-1	5.760-2	6.769-3	3.366-4
5	5	2.040-3	3.522-2	1.320-1	1.210-1	2.726-3	1.592-1	2.007-3	1.945-1	2.501-1	0.693-2	1.207-2
6	6	7.599-4	1.204-2	0.735-2	1.400-1	5.300-2	3.594-2	1.230-1	3.052-2	1.242-1	2.710-1	1.201-1
7	7	2.065-4	3.099-3	2.070-2	9.503-2	1.166-1	1.055-2	7.024-2	7.047-2	7.312-2	6.340-2	2.726-1
8	8	5.700-5	1.239-3	1.110-2	5.000-2	1.091-1	7.590-2	4.770-4	1.041-1	2.602-2	1.090-1	2.176-2
9	9	1.654-5	3.945-4	4.006-3	2.294-2	7.053-2	1.024-1	3.515-2	1.650-2	1.047-1	2.777-3	1.272-1
11	11	4.001-6	1.274-4	1.474-3	9.710-3	3.015-2	0.391-2	0.005-2	0.103-3	4.367-2	0.420-2	2.434-3
11	11	1.477-6	4.192-5	5.299-4	3.947-3	1.051-2	5.370-2	0.665-2	5.170-2	4.042-5	6.743-2	5.395-2
12	12	4.594-7	1.403-5	1.910-4	1.572-3	0.437-3	2.903-2	6.579-2	7.643-2	2.432-2	0.601-3	7.067-2
13	13	1.479-7	4.771-6	7.010-5	6.225-4	3.713-3	1.522-2	4.132-2	7.115-2	5.006-2	6.010-3	2.640-2
14	14	4.944-8	1.647-6	2.593-5	2.471-4	1.602-3	7.372-3	2.393-2	5.235-2	5.022-2	3.620-2	4.695-7
15	15	1.701-8	5.701-7	3.664-5	9.051-5	6.060-4	3.465-3	1.276-2	3.352-2	5.067-2	5.766-2	1.605-2
16	16	5.076-9	2.066-7	3.627-5	3.945-5	2.939-4	1.601-3	0.517-3	1.957-2	4.234-2	5.926-2	4.214-2
17	17	1.962-9	7.493-8	1.371-5	1.504-5	1.250-4	7.330-4	3.241-3	1.091-2	2.740-2	4.003-2	5.379-2
18	18	6.064-10	2.723-8	5.212-7	6.362-6	5.395-5	3.341-4	1.505-3	5.037-3	1.652-2	3.404-2	5.092-2
19	19	1.660-10	9.700-9	1.907-7	2.555-6	2.301-5	1.519-4	7.601-4	3.040-3	9.504-3	2.207-2	4.065-2
21	21	3.079-11	3.279-9	7.522-8	1.024-6	9.799-6	0.079-5	3.696-4	1.557-3	5.294-3	1.415-2	2.912-2

Table 62 (cont'd)

(V2+ MEIVEL)

V	VV	11	12	13	14	15	16	17	18	19	20
5	7.104	-11	2.059-12	1.941-11	7.375-12	1.394-13	3.552-13	1.055-12	2.371-13	1.014-14	0.502-14
6	1.343	-11	1.474-10	2.123-11	1.709-11	2.906-11	2.073-12	4.550-12	5.039-12	7.656-13	3.389-13
1	1.856	-10	1.398-13	1.191-10	5.592-11	2.916-12	3.615-11	1.423-11	2.719-13	7.700-12	5.091-12
2	7.791	-10	9.719-11	3.342-12	1.060-10	9.271-11	1.012-14	3.809-11	2.955-11	7.747-13	7.502-12
3	5.139	-6	1.432-9	6.103-12	7.503-12	5.660-11	9.555-11	3.944-12	2.354-11	3.679-11	7.403-12
4	6.744	-4	1.437-5	3.140-9	3.406-11	3.055-12	4.240-11	9.356-11	1.350-11	1.515-11	4.765-11
5	1.358	-2	1.220-3	2.092-5	3.273-9	2.034-10	2.339-12	2.179-11	7.134-11	1.625-11	0.763-12
6	1.550	-1	2.952-2	2.037-3	3.636-5	1.033-3	9.340-10	1.113-14	3.370-12	4.492-11	1.846-11
7	2.571	-1	1.933-1	4.194-2	3.194-3	5.002-3	3.433-11	1.559-3	0.340-12	3.970-13	1.901-11
8	2.128	-3	2.293-1	2.209-1	5.676-2	4.713-3	9.994-5	3.574-3	2.273-9	5.124-11	1.323-11
9	1.252	-1	2.247-3	1.910-1	2.470-1	7.373-2	5.563-3	1.275-4	2.503-3	2.421-9	1.316-10
10	1.801	-2	1.070-1	1.680-2	1.502-1	2.690-1	9.253-2	9.655-3	1.746-4	9.617-4	1.805-9
11	2.525	-2	4.247-2	7.977-2	3.934-2	1.112-1	2.937-1	1.127-1	1.130-2	2.294-4	2.262-7
12	7.512	-2	5.233-3	0.453-2	5.079-2	5.333-2	7.444-2	2.919-1	1.339-1	1.510-2	2.891-4
13	4.512	-2	5.035-2	6.597-3	7.895-2	2.598-2	0.555-2	4.505-2	2.939-1	1.557-1	1.005-2
14	5.243	-3	5.777-2	3.960-2	5.305-3	9.317-2	9.320-3	1.015-1	2.312-2	2.304-1	1.777-1
15	4.120	-3	1.702-2	6.107-2	2.011-2	1.014-2	7.772-2	0.315-4	1.132-1	0.020-3	2.020-1
16	2.546	-2	1.546-6	3.183-2	5.520-2	5.275-3	3.337-2	6.514-2	1.070-3	1.115-1	1.581-3
17	4.340	-2	1.134-2	3.829-3	4.314-2	4.267-2	2.516-4	4.725-2	4.897-2	7.862-3	1.060-1
18	4.455	-2	3.435-2	2.497-3	1.299-2	4.056-2	2.000-2	1.955-3	5.622-2	3.223-2	1.885-2
19	4.362	-2	4.162-2	1.739-2	3.745-5	2.336-2	4.724-2	1.434-2	9.178-3	5.916-2	1.701-2

Table 63
RKR FRANCK-CONDON FACTORS FOR (N₂⁺ 1ST. NEG.)

v	0	1	2	3	4	5	6	7	8	9	10
0	6.632-1	2.553-1	6.354-2	1.365-2	2.921-3	6.714-4	1.632-4	3.471-5	4.323-6	3.142-8	2.190-7
1	2.895-1	2.385-1	2.856-1	1.290-1	4.170-2	1.130-2	2.025-3	6.692-4	1.487-4	2.639-5	2.446-6
2	4.451-2	3.999-1	5.749-2	2.283-1	1.648-1	7.133-2	2.391-2	6.737-3	1.760-3	3.376-4	1.017-4
3	2.326-3	9.934-2	4.239-1	2.972-3	1.535-1	1.708-1	9.388-2	3.780-2	1.275-2	3.812-3	1.039-3
4	2.017-5	6.363-3	1.607-1	3.940-1	4.415-3	0.794-2	1.357-1	1.079-1	5.111-2	1.996-2	6.915-3
5	3.119-5	6.831-6	1.112-2	2.167-1	3.668-1	1.626-2	4.485-2	1.308-1	1.104-1	6.104-2	2.657-2
6	6.274-7	2.267-5	1.883-5	1.267-2	2.532-1	3.636-1	2.127-2	2.103-2	1.063-1	1.056-1	6.646-2
7	1.868-7	1.652-9	1.166-4	5.437-4	9.335-3	2.711-1	3.735-1	1.657-2	7.935-3	0.825-2	9.680-2
8	8.661-8	1.552-7	7.991-8	2.395-4	2.394-3	3.090-3	2.644-1	4.293-1	5.663-3	1.633-3	7.612-2
9	1.991-7	2.410-10	1.669-5	1.101-5	2.100-4	5.316-3	4.236-4	2.280-1	4.959-1	6.165-5	3.216-5
10	3.812-8	4.435-7	4.256-10	5.051-6	8.128-5	1.975-3	1.879-2	1.563-2	1.380-1	5.501-1	1.354-2
11	5.245-11	4.420-7	9.099-11	1.995-5	4.237-7	2.431-4	4.886-4	9.057-3	5.716-2	4.190-2	5.430-1
12	7.842-9	4.969-8	1.530-7	1.964-8	5.240-6	1.499-3	2.747-4	3.675-4	2.409-3	1.098-1	7.799-4
13	5.090-9	3.200-8	2.524-7	4.072-8	1.312-6	4.346-5	1.583-4	2.035-7	8.286-3	3.039-3	1.162-1
14	2.000-9	1.169-7	5.930-9	3.469-9	2.949-8	4.834-5	4.144-6	3.116-4	1.131-3	7.378-3	3.603-2
15	1.149-9	8.782-8	1.713-9	2.101-8	4.931-8	7.436-7	7.024-6	1.233-4	6.573-5	5.427-3	3.156-4
16	1.135-9	2.668-8	1.499-7	2.994-8	7.129-8	1.117-10	6.631-6	4.132-5	2.995-4	4.038-4	7.830-3
17	1.011-9	1.375-9	1.951-7	9.192-10	3.072-8	5.838-8	1.129-6	6.092-6	1.175-4	1.020-4	4.060-3
18	4.775-11	1.566-9	1.113-7	2.988-8	4.789-9	5.383-8	4.952-9	8.712-6	7.465-5	2.953-4	3.663-4
19	2.340-11	4.343-9	2.305-9	1.332-7	1.276-10	3.350-9	2.224-7	2.935-6	3.533-6	1.358-4	7.805-5
20	1.690-10	3.625-9	1.924-10	1.225-7	2.926-10	2.275-9	1.765-7	1.789-7	8.966-6	1.794-5	2.661-4

(V2-15T. VE9.)

76

Table 64

RKR FRANK-CONDON FACTORS FOR N₂ 2ND. VES.)

V	VV	0	1	2	3	4	5	6	7	8	9	10										
0	1.317-	2	7.594-	2	1.916-	1	2.756-	1	2.461-	1	1.390-	1	4.009-	2	9.165-	3	7.006-	4	2.051-	6	3.453-	6
1	4.864-	2	1.565-	1	1.568-	1	2.726-	2	3.101-	2	1.002-	1	2.311-	1	1.251-	1	3.142-	2	2.775-	3	4.000-	6
2	9.626-	2	1.530-	1	2.608-	2	3.861-	2	1.177-	1	1.033-	2	5.685-	2	2.249-	1	1.969-	1	5.443-	2	6.353-	3
3	1.354-	1	0.345-	2	7.956-	3	9.668-	2	1.269-	2	5.560-	2	0.233-	2	1.420-	3	1.035-	1	2.455-	1	1.037-	1
4	1.517-	1	1.921-	2	0.110-	2	4.213-	2	2.441-	2	6.095-	2	1.957-	3	9.034-	2	1.370-	2	9.465-	2	2.640-	1
5	1.444-	1	1.732-	4	0.160-	2	1.641-	4	6.093-	2	3.072-	3	5.255-	2	2.128-	2	5.306-	2	4.622-	2	4.257-	2
6	1.217-	1	1.862-	2	5.300-	2	2.367-	2	3.927-	2	2.337-	2	3.703-	2	5.408-	2	4.572-	2	1.669-	2	6.069-	2
7	9.342-	2	4.036-	2	1.579-	2	5.504-	2	2.400-	3	5.443-	2	3.709-	5	5.408-	2	2.747-	4	5.017-	2	5.394-	4
8	6.680-	2	6.094-	2	1.302-	4	5.474-	2	9.301-	3	3.360-	2	2.469-	2	1.003-	2	3.610-	2	9.061-	3	4.606-	2
9	4.540-	2	7.519-	2	7.304-	3	3.094-	2	3.524-	2	4.116-	3	4.400-	2	0.993-	4	3.929-	2	1.040-	2	2.060-	2
10	2.953-	2	6.934-	2	2.417-	2	0.444-	3	4.553-	2	3.407-	3	2.056-	2	2.336-	2	7.520-	3	3.008-	2	4.252-	6

V	VV	11	12	13	14	15	16	17	18	19	20		
0	2.009-	7	3.233-	0	4.612-	9	7.976-10	7.062-11	3.937-11	2.001-13	2.099-12	1.213-13	5.610-14
1	2.136-	5	7.448-	7	3.167-	7	1.709-	0	1.392-10	4.274-10	4.922-12	1.401-11	3.169-12
2	1.421-	6	7.215-	5	1.090-	0	1.505-	6	5.297-	6	1.990-	9	1.919-10
3	1.117-	2	3.417-	6	1.756-	4	5.262-	7	2.435-10	1.717-	6.990-	9	4.000-
4	1.452-	1	1.574-	2	5.055-	5	3.435-	4	1.307-	5	3.710-	7	5.619-
5	2.719-	1	1.834-	1	2.271-	2	2.123-	4	5.356-	5	1.320-	6	5.311-
6	1.261-	2	2.614-	1	2.261-	1	2.062-	2	0.340-	4	2.934-	5	4.004-
7	7.201-	2	9.459-	4	2.430-	1	2.637-	1	1.213-	3	9.636-	5	3.692-
8	4.662-	3	0.242-	2	1.351-	3	2.203-	1	3.937-	2	1.250-	3	2.421-
9	2.510-	2	1.995-	2	4.470-	2	0.254-	3	1.937-	1	3.133-	3	1.103-
10	3.989-	2	7.051-	3	3.209-	2	2.612-	2	1.573-	1	5.630-	2	3.095-

Table 65

R-R FRANK-CONDON FACTORS FOR NO GAMMA (1/2)

VV	0	1	2	3	4	5	6	7	8	9	10	11
V												
1	1.605-1	2.611-1	2.397-1	1.014-1	9.156-2	4.543-2	2.214-2	9.614-3	3.932-3	1.538-3	5.947-4	2.320-4
1	3.322-1	1.070-1	5.730-4	7.110-2	1.302-1	1.317-1	3.318-2	5.197-2	3.396-2	1.702-2	8.120-3	3.784-3
2	2.927-1	1.423-2	1.544-1	7.324-2	5.478-4	3.313-2	9.552-2	1.047-1	8.938-2	6.329-2	3.949-2	2.283-2
3	1.501-1	1.931-1	4.735-2	3.774-2	1.115-1	5.141-2	7.533-4	2.133-2	6.297-2	8.344-2	7.901-2	0.211-2
4	5.043-2	2.413-1	4.005-2	1.235-1	2.436-3	5.401-2	8.732-2	3.443-2	2.436-4	1.721-2	4.987-2	0.987-2
5	1.100-2	1.344-1	2.101-1	8.321-4	1.039-1	4.750-2	4.139-3	6.275-2	5.713-2	2.135-2	1.441-7	1.577-2
VV	12	13	14	15	16	17	18	19	20	21	22	23
V												
1	9.034-5	3.667-2	1.585-5	7.448-6	3.749-5	1.455-6	9.113-7	2.475-7	2.520-8	9.361-9	6.653-8	1.015-7
1	1.705-3	7.574-4	3.397-4	1.539-4	6.970-5	2.394-5	1.158-5	3.955-5	1.054-5	1.474-7	9.943-9	3.850-9
2	1.224-2	3.183-3	3.010-3	1.431-3	6.735-4	3.043-4	1.377-4	5.985-5	2.437-5	9.239-6	3.144-6	8.744-7
3	4.200-2	2.552-2	1.451-2	7.477-3	4.161-3	2.111-3	1.032-3	4.939-4	2.273-4	1.123-4	4.484-5	1.421-5
4	6.969-2	5.652-2	4.016-2	2.000-2	1.597-2	9.234-3	5.176-3	2.715-3	1.371-3	6.767-4	3.296-4	1.542-4
5	4.240-2	5.894-2	5.000-2	5.034-2	3.859-2	2.041-2	1.556-2	1.032-2	5.639-3	3.155-3	1.722-3	9.183-4

Table 66

RKR FRANCK-CONDON FACTORS F32 (NO 5A44A (3/2))

V	0	1	2	3	4	5	6	7	8	9	10	11
0	1.511-1	2.516-1	2.346-1	1.674-1	9.994-2	5.235-2	2.457-2	1.074-2	4.406-3	1.746-3	6.925-4	2.010-4
1	3.261-1	1.106-1	7.001-1	5.050-2	1.243-1	1.316-1	1.021-1	5.530-2	3.744-2	1.935-2	9.396-3	4.350-3
2	2.975-1	9.639-3	1.454-1	0.214-1	2.465-3	2.526-2	7.035-2	1.024-1	9.275-2	6.702-2	4.334-2	2.517-2
3	1.566-1	1.049-1	3.730-2	2.700-2	1.076-1	5.026-2	2.779-3	1.520-2	5.622-2	0.009-2	0.031-2	6.453-2
4	5.370-2	2.449-1	3.375-2	1.257-1	5.331-3	4.419-2	9.570-2	5.131-2	1.523-3	1.190-2	4.400-2	6.647-2
5	1.240-2	1.432-1	2.136-1	3.034-3	9.301-2	5.400-2	1.337-3	5.474-2	6.070-2	2.705-2	5.104-4	1.116-2

V	12	13	14	15	16	17	18	19	20	21	22	23
1	1.196-4	5.251-3	2.346-3	9.520-6	3.530-6	1.125-6	2.792-7	4.730-8	3.761-9	3.573-11	7.604-13	1.104-3
2	1.968-3	0.010-4	3.909-4	1.700-4	0.011-5	3.439-5	1.399-5	4.026-6	1.300-6	2.025-7	2.743-9	1.037-3
3	1.361-2	5.996-3	3.467-3	1.600-3	7.737-4	3.541-4	1.650-4	7.150-5	2.037-5	1.012-5	2.030-6	5.349-7
4	4.490-2	2.021-2	1.646-2	0.995-3	4.690-3	2.332-3	1.174-3	5.631-4	2.520-4	1.160-4	4.920-5	1.935-5
5	6.901-2	5.920-2	4.350-2	2.070-2	1.754-2	1.020-2	5.646-3	3.011-3	1.569-3	7.024-4	3.701-4	1.730-4
	3.753-2	5.603-2	0.096-2	5.333-2	4.053-2	2.033-2	1.024-2	1.100-2	6.490-3	3.623-3	1.945-3	1.016-3

Table 67

RKR FRANK-CONDON FACTORS FOR (NO BETA (1/2))

v	v'	0	1	2	3	4	5	6	7	8	9	10	11
1	1.709-5	2.473-4	1.671-3	7.411-3	2.312-2	5.344-2	3.772-2	1.438-1	1.714-1	1.703-1	1.438-1	9.467-2	
1	1.451-4	1.602-3	9.120-3	3.107-2	7.019-2	1.173-1	1.120-1	7.112-2	1.635-2	2.350-3	4.666-2	1.000-1	
2	6.172-4	5.892-3	2.521-2	6.380-2	9.718-2	8.248-2	2.916-2	2.245-4	3.649-2	8.194-2	6.325-2	1.106-2	
3	1.840-3	1.433-2	4.740-2	8.480-2	7.607-2	2.081-2	2.801-3	4.687-2	6.353-2	1.463-2	4.234-3	5.354-2	
4	4.330-3	2.721-2	6.100-2	7.941-2	2.930-2	8.457-4	4.127-2	5.349-2	9.101-3	1.417-2	5.783-2	3.311-2	
5	9.523-3	4.253-2	7.041-2	4.395-2	1.538-3	2.052-2	5.158-2	3.923-3	1.275-2	5.170-2	1.843-2	5.831-3	
6	1.402-2	5.714-2	6.981-2	1.802-2	7.451-3	4.778-2	2.044-2	4.703-3	4.352-2	1.881-2	5.938-3	4.583-2	
7	2.255-2	6.753-2	5.117-2	1.047-3	3.006-2	3.727-2	3.122-3	3.215-2	2.740-2	1.278-3	3.847-2	1.771-2	
8	3.161-2	7.062-2	2.805-2	4.109-3	4.311-2	1.195-2	1.242-2	3.659-2	1.253-3	2.073-2	2.451-2	2.339-3	
9	4.093-2	6.582-2	9.466-3	1.984-2	3.636-2	1.328-3	3.171-2	1.447-2	9.298-3	3.275-2	3.356-4	2.898-2	
10	4.955-2	5.506-2	6.024-4	3.320-2	1.850-2	8.395-3	3.237-2	1.159-4	2.893-2	1.353-2	1.311-2	2.091-2	
11	5.672-2	4.065-2	1.843-3	3.435-2	3.656-3	2.391-2	1.536-2	4.298-3	2.749-2	2.563-4	2.928-2	3.494-3	
12	6.247-2	2.613-2	1.013-2	3.323-2	3.294-4	3.139-2	2.184-3	2.353-2	1.002-2	1.340-2	1.928-2	4.472-3	
13	6.617-2	1.363-2	2.089-2	2.150-2	7.403-3	2.586-2	1.490-3	2.715-2	3.963-5	2.575-2	2.303-3	2.152-2	
14	6.794-2	4.917-3	2.977-2	9.543-3	1.820-2	1.334-2	1.136-2	1.705-2	6.432-3	2.361-2	2.808-3	2.305-2	
15	6.821-2	5.654-4	3.444-2	1.752-3	2.574-2	2.429-3	2.142-2	4.572-3	1.848-2	6.655-3	1.564-2	8.819-3	
16	6.659-2	4.300-4	3.389-2	1.972-4	2.637-2	1.238-4	2.356-2	2.878-3	2.259-2	2.072-7	2.192-2	3.022-5	
17	6.366-2	3.861-3	2.902-2	4.238-3	2.076-2	4.845-3	1.758-2	5.048-3	1.616-2	5.455-3	1.505-2	5.949-3	
18	5.927-2	9.821-3	2.133-2	1.147-2	1.204-2	1.230-2	9.851-3	1.370-2	5.793-3	1.582-2	4.021-3	1.625-2	
19	5.389-2	1.711-2	1.302-2	1.889-2	4.268-3	1.924-2	1.259-3	1.881-2	1.671-4	1.981-2	6.571-5	1.817-2	

Table 67 (cont'd)

(NO BETA (1/2))

VV	12	13	14	15	16	17	18	19	20	21	22	23
V												
J	5.375-2	2.597-2	1.050-2	3.489-3	0.933-4	1.707-4	2.834-5	5.077-5	0.197-7	1.120-8	1.770-8	2.463-8
1	1.403-1	1.270-1	0.577-2	4.448-2	1.771-2	5.530-3	1.425-3	2.691-4	4.143-5	3.967-6	1.122-9	0.264-9
2	7.902-3	0.663-2	1.261-1	1.337-1	9.468-2	4.899-2	1.919-2	5.549-3	1.107-3	1.753-4	1.502-5	5.337-7
3	7.215-2	2.530-2	1.635-3	5.534-2	1.220-1	1.326-1	9.258-2	4.381-2	1.458-2	3.577-3	5.559-4	4.829-5
4	1.166-4	4.141-2	7.100-2	2.534-2	2.689-3	6.403-2	1.314-1	1.278-1	7.777-2	3.152-2	0.195-3	1.311-3
5	5.002-2	3.453-2	1.550-4	4.489-2	6.668-2	1.485-2	1.154-2	9.022-2	1.434-1	1.148-1	5.371-2	1.500-2
6	1.891-2	0.027-3	5.062-2	2.629-2	3.135-3	5.665-2	5.439-2	2.073-3	3.987-2	1.305-1	1.414-1	0.163-2
7	6.000-3	4.434-2	1.175-2	1.381-2	5.187-2	1.155-2	1.555-2	6.795-2	2.858-2	6.194-3	9.555-2	1.565-1
8	3.027-2	1.083-2	1.400-2	4.138-2	2.177-3	2.973-2	4.326-2	1.015-4	4.497-2	5.007-2	1.492-3	5.592-2
9	1.703-2	7.287-3	3.666-2	1.929-3	2.797-2	2.833-2	1.920-3	4.679-2	1.874-2	1.306-2	6.784-2	1.929-2
10	6.005-4	3.265-2	0.197-3	1.957-2	2.716-2	1.747-3	4.000-2	0.382-3	2.199-2	4.320-2	2.704-8	5.337-2
11	2.114-2	1.666-2	7.476-3	2.997-2	1.490-5	3.261-2	9.712-3	1.895-2	3.192-2	1.561-3	4.737-2	1.050-2
12	2.706-2	1.953-5	2.845-2	3.587-3	2.233-2	1.531-2	1.021-2	3.049-2	5.806-4	3.948-2	5.022-3	3.047-2
13	0.001-3	1.471-2	1.622-2	7.356-3	2.441-2	1.403-3	3.087-2	4.525-4	2.996-2	7.352-3	2.293-2	2.311-2
14	4.884-4	2.480-2	1.505-4	2.470-2	2.195-3	2.244-2	7.192-3	1.795-2	1.535-2	1.121-2	2.520-2	4.467-3
15	1.274-2	1.214-2	9.599-3	1.558-2	6.744-3	1.978-2	3.717-3	2.414-2	1.229-3	2.777-2	6.231-5	3.119-2
16	2.168-2	2.403-4	2.157-2	6.540-4	2.168-2	1.498-3	2.150-2	2.775-3	2.139-2	4.556-3	2.135-2	7.102-3
17	1.470-2	5.955-3	1.483-2	5.981-3	1.514-2	5.369-3	1.531-2	5.891-3	1.753-2	5.889-3	1.880-2	6.071-3
18	2.870-3	1.703-2	2.056-3	1.789-2	1.371-3	1.890-2	3.893-4	2.023-2	6.749-4	2.157-2	2.709-4	2.332-2
19	6.841-4	1.721-2	1.820-3	1.590-2	3.436-3	1.454-2	5.144-3	1.324-2	7.439-3	1.144-2	1.068-2	9.306-3

Table 68

RNR FRANCK-CONDON FACTORS FOR (NO 3E1A (3/2))

v	0	1	2	3	4	5	6	7	8	9	10	11
1	1.910-5	2.634-4	1.853-3	7.930-3	2.420-2	5.023-2	1.008-1	1.441-1	1.713-1	1.705-1	1.303-1	9.211-2
2	1.558-4	1.016-3	3.333-3	3.274-2	7.133-2	1.039-1	1.115-1	5.338-2	1.333-2	3.273-3	4.947-2	1.120-1
3	0.594-4	5.335-3	2.727-2	0.609-2	9.699-2	0.132-2	2.347-2	5.932-4	3.973-2	4.170-2	5.939-2	4.939-3
4	1.956-3	1.519-2	5.133-2	0.537-2	7.292-2	1.020-2	4.078-3	4.934-2	6.248-2	1.620-2	5.708-2	5.655-2
5	4.582-3	2.856-2	7.000-2	7.762-2	2.630-2	1.641-3	4.399-2	5.156-2	6.295-3	1.650-2	5.033-2	3.023-2
6	3.976-3	4.427-2	7.857-2	4.633-2	6.770-4	2.345-2	3.462-2	7.723-3	1.510-2	5.067-2	1.500-2	7.746-3
7	1.533-2	5.077-2	7.034-2	1.530-2	9.554-3	4.055-2	1.760-2	5.335-3	4.452-2	1.623-2	7.711-3	4.051-2
8	2.355-2	0.800-2	4.302-2	3.095-4	3.260-2	3.512-2	2.045-3	3.432-2	2.400-2	2.290-3	3.976-2	1.520-2
9	3.200-2	7.033-2	2.575-2	5.740-3	4.355-2	9.002-3	1.521-2	3.573-2	5.134-4	2.877-2	2.211-2	3.030-3
10	4.230-2	6.523-2	7.637-3	2.171-2	3.400-2	7.731-5	3.362-2	1.210-2	1.152-2	3.150-2	3.479-5	3.555-2
11	5.116-2	5.371-2	1.943-4	3.540-2	1.610-2	1.139-2	3.133-2	1.233-6	3.033-2	0.376-3	1.534-2	2.547-2
12	5.034-2	3.047-2	2.448-3	3.001-2	2.376-3	2.556-2	1.393-2	1.056-2	2.607-2	0.428-4	2.971-2	2.210-3
13	6.752-2	2.420-2	1.222-2	3.102-2	9.109-4	3.130-2	1.095-3	2.530-2	7.994-3	1.560-2	1.732-2	6.130-3
14	6.903-2	1.240-2	2.336-2	1.910-2	9.402-3	2.407-2	2.710-3	2.631-2	4.635-5	2.629-2	1.204-3	2.303-2
15	6.903-2	3.917-3	3.130-2	7.301-3	2.026-2	1.121-2	1.364-2	1.513-2	0.352-3	1.909-2	4.244-3	2.234-2
16	0.096-2	2.497-4	3.409-2	7.900-2	2.691-2	1.001-3	2.204-2	3.056-3	2.017-2	4.312-3	1.746-2	7.023-3
17	6.697-2	0.347-4	3.317-2	7.900-2	2.599-2	5.217-4	2.327-2	2.635-4	2.254-2	1.591-4	2.194-4	5.019-3
18	6.365-2	4.927-3	2.730-2	6.091-3	1.922-2	6.334-3	1.504-2	5.932-3	1.451-2	7.170-3	1.346-2	7.072-3
19	5.009-2	1.142-2	1.924-2	1.305-2	1.015-2	1.450-2	5.262-3	1.350-2	4.247-3	1.646-2	2.735-3	1.752-2
20	5.319-2	1.905-2	1.039-2	2.694-2	2.902-3	2.007-2	3.259-4	1.940-2	9.930-5	1.067-2	4.116-4	1.765-2

Table 68 (cont'd)

(40 BETA (3/2))

VV	12	13	14	15	16	17	18	19	20	21	22	23
1	5.192-2	2.453-2	9.732-2	3.173-3	8.217-4	1.621-4	2.795-5	4.223-6	2.577-7	5.505-9	2.020-8	1.234-10
2	1.425-1	1.231-1	8.173-2	4.147-2	1.696-2	5.246-3	1.243-3	2.339-4	3.610-5	3.894-6	7.242-8	1.534-8
3	1.001-2	7.136-2	1.200-1	1.317-1	9.261-2	4.651-2	1.778-2	5.133-3	1.070-3	1.644-4	1.370-5	1.926-7
4	7.391-2	2.190-2	2.873-3	3.995-2	1.259-1	1.386-1	8.810-2	4.138-2	1.390-2	3.197-3	5.000-4	5.129-5
5	5.933-4	4.535-2	6.937-2	2.136-2	4.328-3	6.339-2	1.323-1	1.250-1	7.401-2	2.896-2	7.749-3	1.352-3
6	5.250-2	3.123-2	7.310-2	4.818-2	6.553-2	1.132-2	1.491-2	9.613-2	1.415-1	1.093-1	5.212-2	1.532-2
7	1.600-2	8.458-3	5.143-2	2.302-2	4.931-3	5.357-2	3.153-2	9.536-4	4.425-2	1.306-1	1.394-1	7.936-2
8	9.332-3	4.473-2	9.229-3	1.665-2	5.176-2	8.874-3	2.826-2	5.917-2	2.439-2	8.301-3	9.742-2	1.531-1
9	3.871-2	8.274-3	1.637-2	4.604-2	1.850-3	3.324-2	4.039-2	5.557-6	4.880-2	5.649-2	9.649-4	5.075-2
10	1.432-2	9.720-3	3.534-2	9.429-4	3.074-2	2.626-2	3.420-3	4.836-2	1.556-2	1.575-2	6.831-2	1.703-2
11	1.456-3	3.320-2	4.311-3	2.198-2	2.470-2	3.234-3	4.457-2	3.918-3	2.555-2	4.155-2	9.529-5	5.496-2
12	2.314-2	1.335-2	3.708-3	2.856-2	3.292-4	3.414-2	5.543-3	2.232-2	2.943-2	2.722-3	4.830-2	9.327-3
13	2.576-2	3.737-4	2.910-2	2.255-3	2.437-2	1.278-2	1.272-2	3.832-2	1.633-3	3.924-2	3.714-3	3.258-2
14	6.087-3	1.699-2	1.337-2	3.309-3	2.240-2	2.744-3	2.378-2	3.515-5	3.166-2	5.573-3	2.516-2	2.173-2
15	1.249-3	2.434-2	4.616-6	2.526-2	1.116-3	2.431-2	5.326-3	2.012-2	1.277-2	1.358-2	2.355-2	3.810-3
16	1.473-2	9.805-3	1.177-2	1.374-2	8.614-3	1.798-2	3.412-3	2.243-2	2.505-3	2.734-2	3.622-4	3.107-2
17	2.180-2	2.151-3	2.133-2	1.713-4	2.211-2	5.937-4	2.271-2	1.513-3	2.301-2	3.199-3	2.278-2	5.813-3
18	1.294-2	7.743-3	1.209-2	7.705-3	1.326-2	7.876-3	1.432-2	7.747-3	1.551-2	7.626-3	1.727-2	7.637-3
19	1.781-3	1.812-2	1.023-3	1.884-2	6.043-4	1.959-2	3.394-4	2.054-2	1.338-4	2.212-2	3.544-5	2.378-2
20	1.517-3	1.613-2	3.051-3	1.403-2	4.088-3	1.232-2	5.901-3	1.134-2	9.411-3	9.858-3	1.213-2	7.968-3

Table 69

K22 FRANK-CONJON FACTORS FOR (NO DE-IA (1/2))

VV	0	1	2	3	4	5	6	7	8	9	10	11
V												
J	1.619-1	2.013-1	2.405-1	1.020-1	9.149-2	4.623-2	2.121-2	3.855-3	3.412-3	1.219-3	4.150-4	1.357-4
1	3.438-1	1.032-1	1.499-3	7.544-2	1.334-1	1.303-1	3.547-2	5.729-2	2.978-2	1.384-2	5.964-3	2.427-3
2	3.041-1	2.575-2	1.518-1	6.049-2	1.535-4	4.495-2	3.706-2	1.055-1	6.457-2	5.468-2	3.097-2	1.595-2
3	1.410-1	2.401-1	2.553-2	6.282-2	1.096-1	3.141-2	1.327-3	3.939-2	9.017-2	8.147-2	7.242-2	3.001-2
4	3.757-2	2.481-1	9.756-2	9.932-2	2.755-3	8.148-2	7.173-2	1.093-2	5.934-3	4.279-2	7.227-2	7.734-2
VV	12	13	14	15	16	17	18	19	20	21	22	23
J												
1	4.132-5	1.192-5	3.367-6	9.748-7	2.944-7	7.713-8	5.448-9	9.033-9	6.253-8	1.322-7	1.759-7	1.526-7
2	9.113-4	3.203-4	1.067-4	3.208-5	8.392-5	1.273-5	2.310-9	3.158-7	7.051-7	7.485-7	6.444-7	4.123-7
3	7.304-3	3.081-3	1.175-3	4.051-4	1.223-4	2.692-5	3.973-6	7.935-9	8.084-7	1.729-8	1.967-6	1.659-6
4	2.921-2	1.501-2	6.955-3	2.928-3	1.115-3	3.641-4	3.485-5	1.620-5	5.124-7	1.025-6	3.343-6	4.432-6
5	6.270-2	4.191-2	2.429-2	1.250-2	5.834-3	2.455-3	9.894-4	2.659-4	5.448-5	3.457-6	1.171-6	6.561-6

Table 70

RKR FRANCK-CONDON FACTORS F₃₂ (NO DELTA (3/2))

VV	0	1	2	3	4	5	6	7	8	9	10	11
1	1.524-1	2.52+-1	2.354-1	1.68J-1	9.995-2	5.145-2	2.37+-2	9.985-3	3.661-3	1.434-3	4.947-4	1.723-4
2	3.427-1	1.125-1	1.604-4	6.357-2	1.279-1	1.314-1	3.898-2	6.151-2	3.315-2	1.598-2	7.056-3	2.879-3
3	3.098-1	1.934-2	1.544-1	6.998-2	2.113-4	3.611-2	8.934-2	1.055-1	8.828-2	5.951-2	3.466-2	1.798-2
4	1.478-1	2.335-1	3.359-2	4.989-2	1.093-1	3.048-2	3.850-3	3.202-2	7.443-2	8.814-2	7.582-2	5.323-2
5	4.024-2	2.545-1	8.399-2	1.085-1	5.568-4	7.263-2	7.556-2	1.633-2	2.699-3	3.549-2	6.785-2	7.664-2

VV	12	13	14	15	16	17	18	19	20	21	22	23
1	6.021-3	2.075-5	6.566-6	1.599-6	1.839-7	5.692-9	1.179-7	1.690-7	1.452-7	8.807-8	4.115-8	1.573-8
2	1.095-3	3.922-4	1.325-4	4.093-5	1.081-5	1.312-6	3.950-8	2.473-7	7.347-7	9.389-7	8.240-7	5.596-7
3	8.437-3	3.617-3	1.420-3	5.020-4	1.576-4	4.159-5	7.223-6	2.119-7	6.628-7	2.153-8	2.843-6	2.623-6
4	3.213-2	1.710-2	3.242-3	3.535-3	1.355-3	4.559-4	1.237-4	2.259-5	1.052-5	1.064-6	4.032-6	5.476-6
5	6.511-2	4.56J-2	2.757-2	1.453-2	5.878-3	2.983-3	1.358-3	3.253-4	7.211-5	6.461-6	6.609-7	6.374-6

Table 71

RKR FRANK-CONDON FACTORS FOR (NO EPSILON (1/2))

V	V'	1	2	3	4	5	6	7	8	9	10	11							
1	1.620-	1	2.572-	1	1.543-	1	9.248-	2	4.944-	2	1.155-	2	5.132-	3	2.177-	3	8.994-	4	3.043-
1	3.365-	1	1.071-	1	4.760-	4	6.499-	2	1.220-	1	1.272-	1	3.490-	2	3.703-	2	1.956-	2	9.841-
2	2.943-	1	1.045-	2	1.015-	1	7.308-	2	0.307-	4	2.032-	2	7.903-	2	9.646-	2	6.309-	2	4.073-
3	1.453-	1	2.113-	1	4.231-	2	4.651-	2	1.142-	1	4.744-	2	7.178-	4	5.902-	2	7.001-	2	7.542-
4	4.398-	2	2.389-	1	5.133-	2	1.303-	1	4.956-	4	6.418-	2	8.728-	2	5.735-	2	1.921-	2	4.995-
5	9.195-	3	1.196-	1	2.111-	1	6.092-	4	1.235-	1	4.515-	2	9.534-	3	6.523-	2	1.746-	2	2.503-
6	1.584-	3	3.618-	2	1.730-	1	1.039-	1	5.436-	2	5.259-	2	3.325-	2	3.094-	2	7.092-	2	4.014-
7	2.409-	4	1.434-	3	4.034-	2	1.931-	1	1.975-	2	1.173-	1	1.939-	3	4.564-	2	1.677-	3	4.746-
V	V'	12	13	14	15	16	17	18	19	20	21	22	23						
1	1.408-	4	5.330-	5	2.055-	6	1.567-	6	5.756-	7	1.231-	7	9.730-10	8	4.359-	8	1.202-	7	1.030-
1	2.225-	3	9.077-	4	4.244-	5	2.558-	5	0.003-	5	1.944-	5	2.334-	9	3.353-	9	1.336-	7	2.735-
2	1.339-	2	5.559-	3	3.334-	3	2.027-	4	1.062-	4	3.542-	5	9.294-	6	1.436-	6	9.417-10	4	4.842-
3	4.131-	2	2.544-	2	1.450-	3	1.030-	3	0.290-	4	3.331-	4	1.142-	5	3.064-	5	4.321-	5	3.970-
3	6.758-	2	5.431-	2	3.033-	2	0.044-	3	4.065-	3	1.030-	3	7.015-	4	2.750-	4	7.242-	5	8.653-
5	4.716-	2	5.101-	2	0.017-	2	2.329-	2	1.365-	2	7.303-	3	3.536-	4	1.529-	4	5.091-	4	1.559-
6	1.065-	3	2.208-	2	4.650-	2	4.552-	2	3.223-	2	2.059-	2	1.170-	3	5.998-	3	2.737-	3	1.065-
7	2.998-	2	2.403-	3	5.119-	2	5.650-	2	5.100-	2	4.076-	2	2.731-	2	1.721-	2	9.048-	3	4.715-

Table 72 RK2 FRANK-CONDOM FACTORS ϵ_{32} (NO EPSILON (3/2))

V	VV	0	1	2	3	4	5	6	7	8	9	10	11
0	1.526-1	2.481-1	2.292-1	1.646-1	1.036-1	5.446-1	5.446-2	2.718-2	1.275-2	5.690-3	2.452-3	1.040-3	4.368-4
1	3.323-1	1.161-1	1.114-5	5.396-2	1.169-1	1.257-1	1.257-1	1.014-1	6.014-2	4.049-2	2.292-2	1.126-2	5.479-3
2	3.035-1	1.303-2	1.515-1	8.259-2	2.999-3	2.141-2	2.141-2	7.121-2	9.539-2	8.914-2	6.725-2	4.443-2	2.665-2
3	1.526-1	2.034-1	5.155-2	3.463-2	1.110-1	5.030-2	5.030-2	2.633-3	1.419-2	5.275-2	7.636-2	7.652-2	6.228-2
4	4.695-2	2.433-1	4.127-2	1.355-1	2.621-3	5.330-2	5.330-2	9.728-2	3.766-2	1.029-3	1.294-2	4.432-2	6.540-2
5	9.913-3	1.241-1	2.065-1	3.540-3	1.172-1	5.369-2	5.369-2	4.730-3	6.494-2	5.820-2	2.307-2	5.673-5	1.431-2
6	1.670-3	3.063-2	1.066-1	9.517-2	6.632-2	4.115-2	4.115-2	1.024-1	1.020-2	2.254-2	6.685-2	5.064-2	1.259-2
7	2.938-4	3.695-3	8.799-2	1.093-1	1.224-2	1.211-1	1.211-1	3.013-3	9.033-2	5.450-2	1.117-4	3.946-2	8.185-2

V	VV	12	13	14	15	16	17	18	19	20	21	22	23
0	1.022-4	7.502-5	2.906-5	1.097-5	3.549-6	9.303-7	1.555-7	6.175-3	5.431-9	1.661-8	1.855-8	1.682-8	
1	2.555-3	1.151-3	5.018-4	2.092-4	0.314-5	3.097-5	1.036-5	2.520-5	3.233-7	5.199-9	1.099-7	3.748-7	
2	1.481-2	7.745-3	3.047-3	1.906-3	0.056-4	3.421-4	1.327-4	4.513-5	1.235-5	1.653-6	1.117-8	8.756-7	
3	4.404-2	2.803-2	1.643-2	0.899-3	4.517-3	2.174-3	3.577-4	3.924-4	1.337-4	3.913-5	5.530-6	1.946-8	
4	6.775-2	5.704-2	4.175-2	2.720-2	1.610-2	0.908-3	4.631-3	2.169-3	9.321-4	3.393-4	9.440-5	1.351-5	
5	4.130-2	5.971-2	6.160-2	5.187-2	3.001-2	2.525-2	1.518-2	8.367-3	4.171-3	1.846-3	6.928-4	1.974-4	
6	4.108-4	1.752-2	4.238-2	5.667-2	5.647-2	4.741-2	3.471-2	2.270-2	1.340-2	7.084-3	3.250-3	1.262-3	
7	3.501-2	5.133-3	2.505-3	2.133-2	4.391-2	5.518-2	5.337-2	4.322-2	3.098-2	1.959-2	1.097-2	5.391-3	

Table 73

RKR FRANCK-CONDON FACTORS FOR (V) BETA-PYRINE (1/21)

V	0	1	2	3	4	5	6	7	8	9	10	11
1	2.021-2	0.723-2	1.747-2	1.2362-1	2.164-1	1.433-1	7.379-2	3.332-2	9.897-3	2.593-3	5.436-4	9.753-5
2	6.573-2	1.636-1	1.373-1	2.977-2	9.902-3	1.019-3	1.742-1	1.532-1	9.599-2	4.350-2	1.204-2	3.424-3
3	1.165-1	1.375-1	1.035-2	3.120-2	1.104-1	5.559-2	1.129-4	5.511-2	1.505-1	1.536-1	9.024-2	4.313-2
4	1.505-1	0.146-2	1.174-2	9.109-2	2.092-2	1.640-2	9.275-2	3.333-2	9.670-2	0.420-2	1.405-1	1.419-1
5	1.592-1	7.729-3	5.431-2	4.535-2	9.315-3	7.710-2	1.939-2	2.124-2	0.714-2	3.045-2	2.941-3	7.033-2
6	1.453-1	4.400-3	7.909-2	0.093-4	6.016-2	2.447-2	1.303-2	5.021-2	5.996-3	3.760-2	0.177-2	1.033-2

V	12	13	14	15	16	17	18	19	20	21	22	23
1	1.496-5	1.217-0	3.377-0	9.900-0	5.363-0	3.092-0	1.073-0	3.733-0	0.714-1	2.411-0	3.372-9	6.397-9
2	7.970-4	1.340-4	2.007-5	3.463-6	3.260-7	2.416-0	2.764-0	4.516-0	1.050-0	4.250-0	3.001-1	3.249-0
3	1.419-2	3.640-3	7.925-4	1.370-4	1.532-5	6.050-7	2.500-0	5.236-0	2.194-0	3.991-0	5.735-9	1.949-3
4	8.526-2	3.734-2	1.194-2	2.913-3	5.270-4	6.750-5	5.593-6	5.953-7	1.064-7	3.750-0	2.739-4	6.437-3
5	1.459-1	1.297-1	7.240-2	2.943-2	0.050-3	1.710-3	2.032-4	3.415-5	5.211-6	5.533-7	6.933-1	0.957-3
6	1.440-0	1.014-1	1.400-1	1.110-1	5.395-2	1.044-2	4.732-3	0.944-4	1.303-4	1.933-5	1.703-6	0.107-0

Table 74

RNR FRANK-CONDON FACTORS FOR (NO BETA PRIME (3/2))

V	0	1	2	3	4	5	6	7	8	9	10	11
0	2.122-2	9.000-2	1.071-1	2.371-1	2.106-1	1.439-1	7.141-2	2.730-2	0.972-3	2.470-3	5.002-4	9.330-5
1	6.041-2	1.633-1	1.363-1	2.510-2	1.323-2	1.095-2	1.757-1	1.546-1	9.345-2	4.202-2	1.424-2	3.043-3
2	1.202-1	1.355-1	1.099-2	3.633-2	1.112-1	5.200-2	7.352-4	7.001-2	1.522-1	1.524-1	9.470-2	4.137-2
3	1.539-1	5.740-2	1.515-2	3.326-2	2.420-2	2.043-2	9.522-2	4.037-2	5.057-4	6.926-2	1.479-1	1.447-1
4	1.612-1	5.047-3	6.937-2	4.104-2	1.250-2	7.755-2	1.545-2	2.502-2	8.756-2	3.408-2	4.650-3	8.471-2
5	1.455-1	6.196-3	7.947-2	9.027-2	6.272-2	2.020-2	2.463-2	5.710-2	3.020-3	4.195-2	7.975-2	1.433-2

V	12	13	14	15	16	17	18	19	20	21	22	23
0	7.161-6	3.357-7	6.270-7	7.201-8	4.249-8	4.140-9	1.003-9	3.237-10	7.352-9	1.742-11	2.009-9	1.223-3
1	7.110-6	1.039-4	1.947-5	3.910-6	5.613-6	7.743-6	3.745-9	3.117-9	2.650-9	2.251-9	1.370-9	1.534-11
2	1.332-2	3.357-3	6.695-4	1.129-4	1.530-5	0.371-7	5.371-10	0.334-8	4.133-9	3.752-8	1.047-8	6.247-3
3	3.362-2	3.436-2	1.075-2	2.560-3	4.039-4	6.925-5	5.090-6	1.534-7	1.463-7	7.920-6	7.525-9	3.060-11
4	1.444-1	1.260-1	5.062-2	2.633-2	7.500-3	1.592-3	2.420-4	2.610-5	3.039-6	1.200-6	1.203-7	1.023-7
5	1.040-2	1.074-1	1.460-1	1.075-1	5.164-2	1.710-2	4.212-3	7.900-4	1.226-4	1.907-5	2.234-6	3.155-10

Table 75

MAX FRANK-CONJON FACTORS FOR (N) JANNA PRIME (1/21)

N	6	1	2	3	4	5	6	7	8	9	10	11
1	1.913-1	2.795-1	2.320-1	1.441-1	7.795-1	3.975-2	1.935-2	0.975-2	3.923-3	1.599-3	6.144-4	2.144-4
2	3.423-1	5.021-2	5.774-3	9.124-3	1.411-1	1.230-1	3.100-2	5.434-2	2.993-2	1.511-2	7.229-3	3.243-3
3	2.753-1	3.051-2	1.717-1	0.273-1	2.509-4	4.047-4	9.715-2	1.051-1	0.359-2	5.502-2	3.309-2	1.911-2
4	1.366-1	2.101-1	2.953-2	6.679-2	1.173-1	3.034-2	2.910-4	3.352-2	7.366-2	4.553-2	7.412-2	5.457-2
5	4.371-2	2.353-1	5.459-2	1.130-1	9.050-5	7.455-2	0.390-2	2.597-2	1.131-3	2.925-2	6.043-2	7.411-2
6	5.801-3	1.109-1	2.221-1	1.090-4	1.150-1	3.380-2	1.395-2	7.570-2	5.924-2	1.104-2	2.172-3	2.071-2

N	12	13	14	15	16	17	18	19	20	21	22	23
1	7.068-5	2.130-2	5.552-6	1.111-6	6.559-7	4.136-7	2.185-7	7.662-4	1.061-4	6.508-10	0.431-3	
2	1.382-3	5.411-4	2.020-4	2.738-5	1.015-5	3.319-5	1.676-6	0.237-7	4.796-7	3.121-7	1.992-7	
3	3.974-3	4.920-3	2.174-3	3.734-4	1.521-4	5.191-5	2.589-5	1.240-5	5.276-6	3.342-6	1.452-5	
4	6.729-2	2.071-2	1.143-2	2.986-3	1.493-3	5.278-4	2.795-4	1.230-4	5.758-5	2.047-5	1.359-5	
5	5.323-2	5.103-2	3.452-2	1.291-2	7.254-3	3.044-3	1.939-3	9.176-4	4.216-4	1.936-4	0.445-4	
6		5.342-2	5.907-2	3.439-2	2.270-2	1.392-2	0.129-3	4.655-3	2.339-3	1.109-3	5.751-4	

Table 76

RKR FRANK-CONDON FACTORS FOR (VO GAMMA PRIME (3/2))

V	VV	U	1	2	3	4	5	6	7	8	9	10	11
0	1.040-1		2.703-1	2.207-1	1.505-1	8.563-2	4.417-2	2.146-2	9.933-3	4.340-3	1.003-3	7.130-4	6.701-4
1	3.371-1		9.531-2	2.444-3	7.000-2	1.360-1	1.303-1	3.454-2	5.004-2	3.302-2	1.715-2	8.363-3	3.014-3
2	2.010-1		2.352-2	1.644-1	7.209-2	1.334-4	3.743-2	9.351-2	1.041-1	0.720-2	6.030-2	3.724-2	2.112-2
3	1.430-1		2.093-1	3.790-2	4.765-2	1.162-1	4.501-2	0.520-3	2.621-2	5.770-2	0.451-2	7.642-2	5.729-2
4	4.656-2		2.351-1	5.310-2	1.200-1	3.603-4	6.445-2	9.507-2	2.754-2	5.001-5	2.279-2	5.572-2	7.105-2
5	9.574-3		1.223-1	2.191-1	6.130-5	1.104-1	4.005-2	9.113-3	6.921-2	6.336-2	1.603-2	5.376-4	2.099-2

V	VV	12	13	14	15	16	17	18	19	20	21	22	23
0	9.016-5		3.425-5	1.129-5	3.373-6	0.909-7	2.134-7	5.247-8	2.374-3	2.459-8	3.370-8	4.007-8	3.729-8
1	1.624-3		6.490-4	2.473-4	9.030-5	3.250-5	1.107-5	4.436-6	1.701-5	0.177-7	4.345-7	2.616-7	1.051-7
2	1.115-2		5.497-3	2.530-3	1.095-3	4.526-4	1.957-4	7.547-5	3.232-5	1.416-5	6.229-6	2.762-6	1.254-6
3	3.734-2		2.301-2	1.303-2	6.074-3	3.411-3	1.616-3	7.200-4	3.214-4	1.427-4	6.415-5	2.933-5	1.348-5
4	6.042-2		5.410-2	3.790-2	2.407-2	1.427-2	0.070-3	4.333-3	2.175-3	1.050-3	4.910-4	2.227-4	1.011-4
5	4.036-2		6.274-2	0.150-2	5.041-2	3.652-2	2.452-2	1.531-2	9.025-3	5.102-3	2.700-3	1.350-3	6.523-4

Table 77 RKR FRANCK-CONDON FACTORS FOR (NO HEAT)

VV	J	1	2	3	4	5						
V												
0	9.996-	1	2.793-	5	1.961-	4	5.971-	5	6.195-	7	1.038-	7
1	2.129-	5	9.976-	1	1.223-	3	2.543-	4	2.255-	4	2.414-	5
2	1.862-	4	1.090-	3	9.913-	1	6.611-	3	4.939-	4	5.535-	4
3	8.550-	5	2.566-	4	5.732-	3	3.711-	1	2.030-	2	6.335-	4
4	5.431-	0	2.701-	4	5.904-	4	1.714-	2	9.334-	1	4.551-	2

Table 78 2K2 FRANGC-COMMON FACTORS FOR (NO FEAST 1)

VV	0	1	2	3	4	5						
V												
0	9.909-	1	1.130-	4	3.133-	4	1.547-	5	1.541-	5	4.517-	6
1	2.159-	5	9.907-	1	1.107-	4	4.193-	4	4.791-	5	7.452-	6
2	3.078-	4	1.204-	4	9.914-	1	2.156-	5	4.115-	4	1.175-	7
3	1.449-	5	4.201-	4	2.244-	5	3.978-	1	5.140-	4	1.929-	4
4	2.104-	0	6.819-	0	4.122-	4	5.257-	4	9.958-	1	1.614-	3
5	4.705-	6	7.330-	6	2.919-	6	1.037-	4	1.552-	3	9.917-	1
6	1.176-	0	8.656-	6	2.734-	5	2.852-	5	6.498-	5	1.359-	3
7	6.763-1J		4.207-	6	1.635-	5	3.035-	5	4.982-	5	1.593-	3

Table 79
RKR FRANK-CONDON FACTORS FOR (V) FEAST 2)

VV	U	1	2	3	4	5
U	9.962-	2.659-	4.116-	4.854-	2.315-	2.052-
1	2.766-	9.933-	3.171-	3.931-	2.573-	1.536-
2	2.908-	3.315-	9.913-	1.729-	3.833-	2.714-
3	7.787-	1.976-	4.609-	3.872-	1.7415-	1.442-
4	1.075-	3.150-	8.499-	7.224-	9.033-	8.615-
5	2.476-	6.661-	5.343-	1.435-	9.353-	9.932-

Table 80 2K2 FRANCK-CONDON FACTORS FJ2 (NO E - C)

V	VV	J	1	2	3	4
0	0	9.953-1	2.232-3	5.020-4	2.263-4	4.373-9
1	1	2.233-3	9.959-1	5.103-4	2.004-4	3.903-4
2	2	5.353-4	5.357-4	9.371-1	1.103-4	1.573-4
3	3	2.374-4	2.291-4	1.503-4	9.330-1	2.533-3
4	4	0.101-0	4.040-4	2.211-4	3.175-3	9.705-1
5	5	1.239-5	1.003-5	0.094-4	4.494-4	1.454-2

Table 8I RK2 FRANCK-CONDON FACTORS FOR (ND FEAST-HEATH)

V'	0	1	2	3	4	5	6	7								
0	3.455-	1	3.424-	3	1.002-	5	1.891-	5	1.058-	5	9.164-	6	1.342-	8	1.229-	6
1	3.341-	3	9.300-	1	4.633-	3	2.224-	4	1.553-	5	4.381-	7	1.021-	5	5.776-	9
2	1.448-	6	4.501-	3	9.899-	1	4.224-	3	5.245-	4	1.025-	6	1.001-	5	1.012-	7
3	1.297-	2	3.437-	4	3.455-	3	3.315-	1	3.881-	3	1.133-	4	1.304-	7	9.032-	5
4	7.410-	0	1.305-	6	8.365-	4	3.493-	3	9.912-	1	2.366-	3	1.309-	5	1.303-	6
5	8.460-	6	2.354-	7	3.128-	5	5.556-	4	2.697-	3	9.909-	1	2.334-	3	6.140-	4

Table 82

RK2 FRANK-CONJON FACTORS FOR (NO L - M)

V	0	1	2	3	4	5	6	7	8	9	10	11
0	3.521-3	2.233-2	6.036-2	1.362-1	1.924-1	2.034-1	1.654-1	1.134-1	5.954-2	2.662-2	1.013-2	3.242-3
1	1.586-2	6.960-2	1.333-1	1.293-1	5.536-2	7.420-4	3.304-2	1.111-1	1.531-1	1.372-1	9.003-2	4.534-2
2	3.044-2	1.114-1	1.030-1	2.602-2	7.200-3	7.434-2	0.030-2	2.570-2	3.166-3	6.307-2	1.345-1	1.135-1
3	0.636-2	1.132-1	4.125-2	4.430-3	6.023-2	5.647-2	0.347-4	3.091-2	0.373-2	3.057-2	1.045-2	4.421-2
4	9.145-2	0.955-2	1.610-3	4.007-2	5.641-2	3.630-4	4.425-2	3.039-2	3.797-3	2.951-2	7.744-2	3.740-2
5	1.069-1	4.754-2	1.111-2	6.601-2	7.044-3	2.975-2	3.195-2	1.136-3	3.040-2	3.440-2	2.747-3	3.150-2
6	1.096-1	1.469-2	4.074-2	3.907-2	5.914-3	5.326-2	6.306-3	2.770-2	4.549-2	2.153-4	4.117-2	4.531-2
7	1.006-1	0.066-4	5.770-2	0.927-3	3.401-2	2.750-2	0.009-3	4.520-2	2.529-3	3.194-2	3.504-2	6.436-4
V	12	13	14	15	16	17	18	19	20	21	22	23
0	0.602-4	1.724-4	2.513-5	4.710-6	1.251-6	5.497-0	9.237-9	5.750-9	1.999-9	5.346-9	2.554-9	1.070-9
1	1.039-2	5.709-3	1.459-3	3.004-4	5.700-5	1.025-5	0.394-7	2.510-10	0.790-9	4.071-0	5.905-14	2.350-0
2	1.005-1	5.206-2	2.057-2	0.543-3	1.640-3	3.390-4	5.501-5	5.212-6	5.209-7	4.090-7	5.096-9	1.457-7
3	1.212-1	1.364-1	9.760-2	3.669-2	1.931-2	5.714-3	1.351-3	2.547-4	3.931-5	4.211-6	3.707-7	3.563-9
4	1.065-4	5.059-2	1.219-1	1.337-1	0.969-2	4.201-2	1.367-2	4.326-3	9.319-4	1.547-4	2.415-5	3.415-6
5	7.457-2	2.948-2	2.221-3	6.446-2	1.200-1	1.243-1	7.006-2	3.397-2	1.110-2	2.007-3	5.041-4	0.052-5
6	2.496-4	4.132-2	6.976-2	1.606-2	9.971-3	0.362-2	1.349-1	1.120-1	6.334-2	2.620-2	7.000-3	1.782-3
7	4.606-2	3.334-2	1.100-3	5.301-2	5.929-2	5.300-3	2.465-2	1.021-1	1.350-1	1.034-1	5.259-2	1.955-2

Table 83

RKR FRANK-CONDON FACTORS FOR (3(2) 5-2)

VV	0	1	2	3	4	5	6	7	8	9	10	11
3	3.547-3	1.021-7	1.430-6	1.293-5	0.264-5	4.037-4	1.538-3	5.145-3	1.352-2	3.438-2	5.765-2	9.277-2
1	3.449-8	9.091-7	1.142-5	9.071-5	5.105-4	2.107-3	7.154-3	1.075-2	3.910-2	6.537-2	0.637-2	0.593-2
2	2.143-7	5.053-6	5.697-5	4.015-4	1.953-3	7.109-3	1.351-2	4.007-2	0.457-2	5.774-2	2.167-2	
3	9.135-7	1.954-5	1.979-4	1.231-3	5.243-3	1.011-2	3.523-2	5.900-2	5.621-2	4.434-2	1.090-2	1.697-3
4	2.914-6	5.001-5	5.162-4	2.342-3	1.049-2	2.711-2	4.914-2	5.935-2	4.172-2	9.056-3	2.093-3	2.461-2
5	7.663-6	1.361-4	1.113-3	5.419-3	1.726-2	3.713-2	5.255-2	4.372-2	1.390-2	4.503-4	2.222-2	3.347-2
6	1.733-5	2.011-4	2.071-3	0.421-3	2.445-2	4.323-2	4.513-2	2.251-2	5.650-4	1.264-2	3.306-2	4.905-2
7	3.490-5	5.194-4	3.450-3	1.317-2	3.092-2	4.420-2	3.326-2	0.545-3	3.409-3	2.597-2	2.552-2	2.222-3
8	6.299-5	4.594-4	5.173-3	1.744-2	3.490-2	3.942-2	1.091-2	1.395-4	1.355-2	2.764-2	9.543-3	2.026-3
9	1.018-4	1.269-3	6.930-3	2.074-2	3.527-2	3.072-2	7.555-3	2.009-3	2.092-2	1.905-2	6.325-4	1.153-2
10	1.477-4	1.724-3	0.600-3	2.292-2	3.306-2	2.145-2	1.590-3	7.520-3	2.137-2	0.797-3	1.391-3	1.793-2
11	1.963-4	2.130-3	9.709-3	2.331-2	2.047-2	1.314-2	1.037-7	1.219-2	1.776-2	2.101-3	6.439-3	1.607-2
12	2.399-4	2.449-3	1.030-2	2.225-2	2.307-2	7.126-3	3.339-4	1.417-2	1.190-2	2.047-5	1.045-2	1.161-2
13	2.699-4	2.604-3	1.020-2	2.002-2	1.750-2	3.355-3	2.571-3	1.351-2	5.770-3	6.009-4	1.152-2	6.106-3
14	2.017-4	2.501-3	9.579-3	1.711-2	1.299-2	1.333-3	3.013-3	1.155-2	3.330-3	2.051-3	1.027-2	2.572-3
15	2.723-4	2.403-3	3.460-3	1.400-2	9.290-3	4.292-4	4.325-3	9.059-3	1.430-3	3.014-3	0.083-3	7.935-4
16	2.481-4	2.113-3	7.151-3	1.115-2	6.523-3	9.250-5	4.214-3	6.749-3	5.290-4	3.323-3	5.902-3	1.417-4
17	2.125-4	1.760-3	5.764-3	0.542-3	4.505-3	5.022-6	3.694-3	4.039-3	1.619-4	3.110-3	4.101-3	1.667-6
18	1.736-4	1.414-3	4.495-3	6.412-3	3.111-3	3.406-6	3.029-3	3.410-3	3.630-5	2.043-3	2.793-3	2.395-5
19	1.349-4	1.002-3	3.371-3	4.658-3	2.110-3	1.005-5	2.342-3	2.354-3	3.094-5	2.005-3	1.067-3	6.360-5
20	0.005-5	6.991-4	2.147-3	2.900-3	1.253-3	2.134-5	1.519-3	1.410-3	3.432-8	1.367-3	1.090-3	6.390-5

Table 83 (cont'd)

(C)(2) S-2)

VV	12	13	14	15	16	17	18	19	20	21	22	23
0	1.275-1	1.504-1	1.519-1	1.321-1	9.974-2	6.535-2	3.023-2	1.934-2	8.476-3	3.230-3	1.131-3	3.003-4
1	5.050-2	1.973-2	1.965-5	1.946-2	6.021-2	1.143-1	1.311-1	1.153-1	8.112-2	4.730-2	2.301-2	1.090-2
2	9.073-5	1.910-2	5.757-2	7.123-2	4.120-2	4.674-3	9.030-3	5.537-2	1.035-1	1.105-1	1.016-1	7.206-2
3	2.948-2	5.375-2	3.545-2	3.265-3	1.161-2	5.294-2	5.424-2	2.039-2	1.035-4	2.270-2	7.705-2	1.247-1
4	4.399-2	1.953-2	9.064-5	2.553-2	5.030-2	2.562-2	1.540-5	2.713-2	6.101-2	4.450-2	5.579-3	1.261-2
5	1.650-2	4.101-4	2.567-2	3.905-2	1.042-2	4.010-3	3.950-2	4.043-2	5.210-3	1.003-2	5.024-2	5.355-2
6	1.098-5	1.925-2	3.349-2	7.031-3	5.059-3	3.550-2	2.455-2	2.013-5	2.637-2	4.437-2	1.291-2	4.950-3
7	1.010-2	2.951-2	1.079-2	2.027-3	2.093-2	2.053-2	3.670-5	2.641-2	3.250-2	2.565-3	1.407-2	4.147-2
8	2.289-2	1.603-2	5.703-5	2.000-2	2.179-2	1.940-4	1.937-2	2.695-2	1.271-3	1.093-2	3.355-2	5.264-3
9	2.132-2	2.657-3	0.799-3	2.274-2	3.439-3	9.290-3	2.494-2	3.307-3	1.111-2	2.003-2	5.030-3	1.004-2
10	1.125-2	5.031-4	1.753-2	1.120-2	1.162-3	2.005-2	3.571-3	3.071-3	2.396-2	0.444-3	4.573-3	4.537-2
11	2.760-3	0.113-3	1.647-2	1.611-3	9.065-3	1.009-2	1.035-4	1.431-2	1.432-2	2.637-4	1.090-2	1.171-2
12	1.355-5	1.005-2	9.707-3	3.250-4	1.375-2	6.591-3	2.050-3	1.642-2	2.540-3	0.232-3	1.710-2	3.025-4
13	1.061-3	1.161-2	3.703-3	3.265-3	1.222-2	9.511-4	9.039-3	1.040-2	1.033-4	1.370-2	6.924-3	2.603-3
14	2.952-3	9.543-3	7.701-4	5.031-3	7.936-3	0.135-5	3.935-3	4.175-3	3.015-3	1.200-2	0.901-4	7.743-3
15	4.109-3	0.733-3	7.226-6	6.552-3	4.254-3	1.103-3	9.537-3	9.595-4	5.440-3	7.475-3	1.145-4	9.114-3
16	4.315-3	4.341-3	1.040-4	5.921-3	1.939-3	2.100-3	5.191-3	4.037-5	5.900-3	3.763-3	1.220-3	7.607-3
17	3.066-3	2.647-3	4.926-4	4.715-3	7.722-4	2.555-3	4.056-3	9.117-5	5.216-3	1.610-3	2.120-3	5.319-3
18	3.106-3	1.504-3	0.641-4	3.517-3	2.737-4	2.414-3	2.549-3	2.930-4	4.050-3	6.205-4	2.371-3	3.425-3
19	2.424-3	3.462-4	5.741-4	2.502-3	9.452-5	2.011-3	1.555-3	4.135-4	2.942-3	2.130-4	2.142-3	2.112-3
20	1.555-3	5.023-4	5.107-4	1.521-3	2.040-5	1.354-3	9.470-4	3.637-4	1.001-3	6.051-5	1.506-3	1.139-3

Table 84

RKR FRANK-CONDON FACTOR FOR (V2 P-013 1)

v'	v''	1	2	3	4	5	6	7	8	9	10
0	9.039-1	9.274-2	3.310-3	4.414-5	4.072-7	6.050-9	8.334-12	7.035-12	2.122-12	7.692-13	2.349-13
1	0.956-2	7.291-1	1.714-1	9.792-3	1.097-4	2.366-5	4.107-8	6.036-11	7.005-11	2.051-11	7.140-12
2	0.164-3	1.596-1	5.771-1	2.372-1	1.937-2	5.119-4	8.252-6	1.706-7	2.186-10	4.046-10	1.137-10
3	3.635-4	1.709-2	2.130-1	4.454-1	2.910-1	3.202-2	1.110-3	2.241-5	5.340-7	5.525-10	1.565-9
4	1.740-5	1.375-3	3.167-2	2.515-1	3.323-1	3.333-1	4.750-2	2.111-3	5.219-5	1.423-6	1.004-9
5	5.022-7	0.796-5	3.294-3	4.398-2	2.750-1	2.366-1	3.542-1	6.633-2	3.679-3	1.095-4	3.393-6
6	5.933-9	3.996-6	2.666-4	6.337-3	6.021-2	2.899-1	1.576-1	3.030-1	0.771-2	6.015-3	2.129-4
7	2.912-10	9.195-8	1.506-5	6.335-4	1.070-2	0.856-2	2.917-1	9.492-2	3.921-1	1.117-1	9.367-3
8	1.106-10	1.000-10	5.399-7	4.759-5	1.291-3	1.655-2	1.092-1	2.030-1	4.030-2	3.091-1	1.377-1
9	3.046-13	5.140-10	3.199-9	2.391-6	1.197-4	2.347-3	2.460-2	1.232-1	2.649-1	1.767-2	5.750-1
10	2.525-11	2.705-11	0.305-11	5.993-8	0.250-6	2.657-4	3.991-3	3.314-2	1.475-1	2.304-1	2.265-3
11	2.965-11	2.695-10	4.340-10	1.737-9	4.092-7	2.390-5	5.372-4	5.354-3	4.392-2	1.629-1	2.052-1
12	1.942-11	3.151-10	1.655-9	3.639-9	3.037-8	1.020-5	5.066-5	1.009-3	9.092-3	5.620-2	1.744-1
13	1.047-11	2.239-10	1.003-9	7.505-9	2.090-8	2.065-7	0.317-6	1.309-4	1.704-3	1.417-2	6.964-2
14	4.762-12	1.200-10	1.403-9	0.109-9	2.033-8	9.450-8	9.217-7	1.046-5	2.925-4	2.995-3	1.996-2
15	2.242-12	6.710-11	0.625-10	0.302-9	2.900-8	9.397-8	3.550-7	3.245-5	4.750-5	5.745-4	4.910-3
16	1.105-12	3.350-11	4.020-10	4.102-9	2.332-8	9.045-8	2.025-7	1.153-6	9.704-5	1.105-4	1.003-3
17	5.712-13	1.600-11	2.612-10	2.492-9	1.610-8	7.329-8	2.513-7	7.045-7	3.396-6	2.565-5	2.366-4
18	2.909-13	0.692-12	1.414-10	1.430-9	1.020-8	5.273-8	2.032-7	6.474-7	2.037-5	9.020-6	6.147-5
19	1.531-13	4.762-12	7.027-11	0.250-10	6.226-9	3.519-8	1.525-7	5.247-7	1.565-6	4.995-6	2.200-5
20	7.727-14	2.779-12	4.400-11	4.799-10	3.759-9	2.250-8	1.062-7	3.993-7	1.247-6	3.501-6	1.155-5

Table 84 (cont'd)

(V2 PHOTO 1)

V	VV	11	12	13	14	15	16	17	18	19	20
0	5.207-	14	1.270-14	1.015-14	1.016-14	1.017-14	1.018-14	1.019-14	1.020-14	1.022-14	1.024-14
1	2.502-	12	9.375-13	3.443-13	1.151-13	3.938-14	1.040-14	1.154-14	1.021-14	1.023-14	1.025-14
2	4.205-	11	1.595-11	5.012-12	2.207-12	0.977-13	3.958-13	1.079-13	9.038-14	3.002-14	1.241-14
3	4.533-	10	1.791-10	7.040-11	2.709-11	1.151-11	4.950-12	2.190-12	9.631-13	4.061-13	1.546-13
4	4.895-	9	1.455-9	6.060-10	2.537-10	1.066-10	4.577-11	1.935-11	0.720-12	3.762-12	1.535-12
5	1.269-	9	1.327-9	4.090-9	1.770-9	7.739-10	3.372-10	1.481-10	6.573-11	2.055-11	1.101-11
6	7.464-	8	9.620-10	3.221-8	1.013-8	4.533-9	2.134-9	9.245-10	4.114-10	1.016-10	7.007-11
7	3.906-	4	1.544-5	1.213-11	7.136-8	2.270-8	1.047-8	4.938-9	2.231-9	1.004-9	4.353-10
8	1.402-	2	5.841-4	3.038-5	3.111-9	1.468-7	4.640-8	2.258-8	1.034-8	4.705-9	2.153-9
9	1.653-	1	2.032-2	1.153-3	5.736-5	2.055-8	2.039-7	0.755-9	4.252-8	2.015-8	9.274-9
10	3.505-	1	1.934-1	2.060-2	1.002-3	1.046-4	1.330-7	5.194-7	1.545-7	7.593-8	3.573-8
11	1.235-	3	3.104-1	2.210-1	3.925-2	2.936-3	1.031-4	4.539-7	9.041-7	2.525-7	1.249-7
12	1.672-	1	1.303-2	2.744-1	2.466-1	5.259-2	4.622-3	3.197-4	1.370-6	1.505-6	3.053-7
13	1.006-	1	1.269-1	3.537-2	2.265-1	2.685-1	5.039-2	6.992-3	5.351-4	3.598-6	2.308-6
14	0.366-	2	1.013-1	0.729-2	6.513-2	1.757-1	2.031-1	0.028-2	1.035-2	0.773-4	0.530-6
15	2.721-	2	9.745-2	1.729-1	5.175-2	9.043-2	1.254-1	2.943-1	1.106-1	1.501-2	1.402-3
16	7.416-	3	3.591-2	1.099-1	1.500-1	2.356-2	1.310-1	7.929-2	2.948-1	1.356-1	2.130-2
17	1.005-	3	1.101-2	4.591-2	1.190-1	1.302-1	5.551-3	1.577-1	4.123-2	2.053-1	1.624-1
18	4.724-	4	3.113-3	1.577-2	5.602-2	1.255-1	1.009-1	2.594-3	1.747-1	1.457-2	2.663-1
19	1.357-	4	0.969-4	4.990-3	2.191-2	5.796-2	1.250-1	7.051-2	7.214-3	1.705-1	1.444-3
20	5.029-	5	2.703-4	1.575-3	7.653-3	2.909-2	7.029-2	1.196-1	4.076-2	2.593-2	1.673-1

Table 85

RKR FRANCK-CONDON FACTOR FOR (V2 P4013 2)

V	u	1	2	3	4	5	6	7	8	9	10
0	2.726-1	3.027-1	2.360-1	0.499-2	2.000-2	3.265-3	3.845-4	3.336-5	2.061-5	9.331-6	3.346-9
1	3.197-1	2.549-2	1.126-1	2.712-1	1.070-1	6.733-2	1.509-2	2.290-3	2.417-4	1.002-5	9.250-7
2	2.155-1	2.454-2	1.577-1	7.501-5	1.593-1	2.354-1	1.299-1	3.944-2	7.557-3	9.743-4	8.653-5
3	1.110-1	1.504-1	9.210-3	1.345-1	5.290-2	4.216-2	2.094-1	1.050-1	7.622-2	1.043-2	2.076-3
4	4.953-2	1.598-1	3.709-2	0.140-2	4.159-2	1.198-1	5.913-6	1.346-1	2.116-1	1.232-1	3.660-2
5	2.031-2	1.004-1	1.102-1	0.607-4	1.138-1	3.672-3	1.210-1	2.946-2	5.521-2	2.000-1	1.619-1
6	7.625-3	5.959-2	1.237-1	3.487-2	3.950-2	7.658-2	2.555-2	7.127-2	0.056-2	7.201-3	1.556-1
7	2.008-3	2.090-2	9.442-2	0.002-2	3.244-4	0.133-2	2.235-2	7.258-2	1.038-2	1.111-1	3.622-3
8	1.015-3	1.293-2	5.845-2	1.005-1	3.493-2	1.697-2	0.132-2	2.007-5	9.067-2	9.077-5	1.020-1
9	3.641-4	5.513-3	3.103-2	0.145-2	7.451-2	2.724-3	5.250-2	4.755-2	1.044-2	6.992-2	1.959-2
10	1.305-4	2.280-3	1.596-2	5.443-2	0.429-2	3.472-2	6.023-3	7.057-2	1.146-2	5.197-2	3.125-2
11	4.733-5	9.270-4	7.581-3	3.221-2	7.093-2	6.474-2	5.509-3	3.173-2	5.024-2	3.007-4	7.006-2
12	1.739-5	3.736-4	3.470-3	1.753-2	5.000-2	7.223-2	3.372-2	1.495-3	5.463-2	2.050-2	1.649-2
13	6.203-5	1.501-4	1.561-3	9.094-3	3.155-2	5.226-2	5.532-2	0.133-3	1.039-2	5.706-2	4.583-3
14	2.342-5	6.039-5	0.912-4	4.539-3	1.045-2	4.531-2	6.251-2	3.199-2	1.139-4	4.014-2	3.331-2
15	0.851-7	2.440-5	3.030-4	2.210-3	1.024-2	3.053-2	5.531-2	5.029-2	9.614-3	1.044-2	5.023-2
16	3.305-7	9.920-5	1.331-4	1.059-3	5.479-3	1.091-2	4.232-2	5.518-2	2.969-2	6.662-5	2.899-2
17	1.305-7	4.063-6	5.025-5	5.021-4	2.059-3	1.114-2	2.945-2	4.959-2	4.440-2	1.019-2	5.971-3
18	5.040-8	1.676-6	2.555-5	2.306-4	1.466-3	0.335-3	1.910-2	3.921-2	4.079-2	2.698-2	3.006-4
19	1.942-8	6.949-7	1.123-5	1.111-4	7.424-4	3.511-3	1.131-2	2.042-2	4.472-2	3.921-2	9.949-3
20	7.435-9	2.006-7	4.952-5	5.205-5	3.729-4	1.910-3	7.141-3	1.934-2	3.046-2	4.319-2	2.393-2

Table 85 (cont'd)

(V2 PH373 2)

V	VV	11	12	13	14	15	16	17	18	19	20
1	2	543-10	5.137-12	4.259-12	5.291-12	4.372-14	5.251-13	3.745-13	4.152-14	1.027-14	9.006-14
2	3	881-8	1.659-9	6.307-12	6.770-12	2.336-11	3.570-13	5.044-12	2.353-12	7.549-14	8.626-13
3	5	366-6	2.432-7	8.292-9	1.162-11	1.026-14	3.074-11	5.110-12	3.372-12	6.258-12	4.703-13
4	3	015-4	2.153-5	1.083-6	3.064-8	3.400-10	5.631-12	3.983-11	1.019-11	3.251-12	1.093-11
5	6	901-3	8.495-4	7.057-5	3.954-5	1.518-7	2.510-9	5.205-11	3.719-11	1.420-11	8.207-13
6	5	272-2	1.422-2	2.049-3	1.941-4	1.233-5	5.214-7	1.131-8	2.357-10	4.769-11	2.242-11
7	1	909-1	9.501-2	2.602-2	4.300-3	4.754-4	3.334-5	1.586-5	4.150-8	9.148-10	6.189-11
8	9	519-2	1.998-1	1.298-1	4.311-2	8.483-3	1.053-3	0.447-5	4.374-6	1.317-7	2.584-9
9	3	359-2	3.971-2	1.826-1	1.515-1	5.562-2	1.512-2	2.144-3	1.931-4	1.106-5	3.703-7
10	6	412-2	7.330-2	6.165-3	1.450-1	1.841-1	3.259-2	2.536-2	4.051-3	4.104-4	2.584-5
11	5	440-2	2.233-2	9.925-2	1.714-3	9.751-2	1.323-1	1.219-1	3.834-2	7.219-3	8.161-4
12	3	782-3	7.728-2	1.110-3	9.896-2	2.214-2	5.037-2	1.934-1	1.531-1	5.706-2	1.211-2
13	6	353-2	3.258-3	7.392-2	6.722-3	7.453-2	5.452-2	1.515-2	1.579-1	1.736-1	7.920-2
14	4	243-2	3.284-2	2.481-2	4.873-2	3.189-2	3.955-2	0.34-2	3.377-4	1.206-1	1.885-1
15	1	587-3	5.593-2	7.491-3	5.020-2	1.867-2	5.873-2	1.058-2	9.617-2	6.634-3	7.894-2
16	1	473-2	1.770-2	5.025-2	3.402-4	5.159-2	1.244-3	7.131-2	1.958-7	8.808-2	2.843-2
17	4	234-2	7.312-4	3.837-2	2.855-2	1.311-2	5.240-2	4.439-3	6.474-2	9.820-3	6.348-2
18	4	209-2	2.291-2	4.500-3	4.738-2	7.366-3	3.444-2	2.972-2	2.335-2	4.217-2	3.254-2
19	2	116-2	4.112-2	5.266-3	2.076-2	4.038-2	7.736-5	4.895-2	8.125-3	4.486-2	1.678-2
20	3	593-3	3.473-2	2.734-2	2.375-4	3.654-2	2.152-2	9.226-3	4.733-2	9.538-6	5.566-2
21	6	358-4	1.539-2	3.778-2	1.015-2	3.334-3	4.353-2	4.730-3	2.732-2	3.088-2	8.415-3

Table 86

RKR FRANCK-CONDON FACTOR FOR (V2 PHOTO 3)

V	VV	0	1	2	3	4	5	5	7	8	9	10
1	0	0.843-1	1.027-1	1.150-2	1.273-3	1.595-4	2.364-5	4.335-6	9.353-7	2.605-7	9.332-8	2.927-8
1	1	1.131-1	6.054-1	1.567-1	2.343-2	4.510-3	7.237-4	1.323-4	2.831-5	7.536-5	2.297-6	7.068-7
2	2	2.579-3	2.053-1	5.296-1	2.002-1	4.909-2	9.073-3	1.377-3	4.333-4	1.090-4	3.240-5	1.092-5
3	3	3.851-7	6.563-3	2.812-1	4.090-1	2.134-1	6.995-2	1.716-2	4.159-3	1.071-3	3.110-4	1.026-4
4	4	2.518-5	1.260-5	1.093-2	3.448-1	3.171-1	2.030-1	0.752-2	2.555-2	7.439-3	2.215-3	7.243-4
5	5	3.210-3	1.440-5	9.047-5	1.473-2	3.992-1	2.401-1	1.029-1	1.012-1	3.513-2	1.135-2	4.030-3
6	6	1.796-9	3.202-10	4.746-5	3.720-4	1.739-2	4.469-1	1.974-1	1.543-1	1.134-1	4.403-2	1.728-2
7	7	4.214-11	2.466-8	7.227-6	1.134-4	1.130-3	1.013-2	4.094-1	1.613-1	1.200-1	1.150-1	5.140-2
8	8	3.532-14	3.446-11	1.536-7	1.132-6	2.102-4	2.064-3	1.553-2	5.250-1	1.365-1	0.556-2	1.155-1
9	9	9.700-12	1.173-11	6.336-10	6.295-7	7.476-6	3.425-4	5.202-3	1.295-2	5.579-1	1.207-1	5.266-2
10	10	1.506-12	5.711-11	0.754-11	2.033-8	1.040-6	3.322-5	4.256-4	1.237-2	7.434-3	5.790-1	1.110-1
11	11	1.020-14	3.343-11	2.775-10	3.302-10	1.903-7	3.069-5	1.144-4	3.765-4	2.221-2	2.091-3	5.073-1
12	12	1.029-14	6.572-12	2.240-10	4.809-10	4.156-10	1.093-5	5.311-6	3.245-4	1.400-4	3.659-2	9.536-5
13	13	1.743-13	6.510-13	2.959-11	7.595-10	9.030-11	0.239-13	4.573-6	2.042-5	7.790-4	1.026-5	5.522-2
14	14	2.044-13	1.062-14	3.069-14	1.023-10	1.509-9	2.146-3	5.672-8	1.475-5	1.140-6	1.506-3	1.147-3
15	15	1.030-14	4.422-13	4.180-12	5.251-12	2.035-10	3.796-13	3.246-8	7.055-7	3.676-5	6.039-5	2.600-3
16	16	1.400-13	6.323-13	4.337-12	3.725-11	5.631-11	4.646-13	2.235-9	1.542-7	5.012-5	5.650-5	4.264-4
17	17	2.698-13	3.321-13	2.178-12	2.908-11	2.424-10	2.531-13	1.343-10	0.362-9	3.095-7	2.492-5	7.010-5
18	18	7.414-14	3.720-14	5.689-13	1.103-11	1.633-10	1.030-9	5.093-10	4.153-9	6.770-7	4.750-6	9.133-5
19	19	1.340-14	1.091-14	2.405-14	1.912-12	4.437-11	5.322-10	2.424-9	4.145-10	1.072-7	2.920-6	2.064-6
20	20	1.200-13	0.206-14	5.241-14	2.545-14	1.626-12	1.214-10	1.744-9	2.148-9	0.521-10	1.079-6	6.645-6

Table 86 (cont'd)

(V2 PHOTO 3)

V	VV	11	12	13	14	15	16	17	18	19	20
0	1.024-	0	3.035-	9	5.005-10	2.210-10	9.131-11	3.261-11	1.553-11	0.057-12	5.100-12
1	2.912-	7	1.131-	7	1.052-	8	3.332-	9	6.373-10	2.004-10	1.344-11
2	4.066-	6	1.020-	6	2.095-	7	3.555-	8	1.134-	5.552-	2.659-
3	3.792-	5	1.523-	5	2.900-	6	3.132-	7	1.610-	6.005-	3.421-
4	2.664-	4	1.173-	4	2.127-	5	4.095-	5	1.219-	6.145-	3.169-
5	1.407-	3	5.905-	4	1.215-	4	2.972-	5	7.952-	4.211-	2.256-
6	6.037-	3	2.729-	3	5.052-	4	1.435-	4	4.133-	2.306-	1.204-
7	2.343-	2	1.030-	2	2.196-	3	3.935-	4	1.916-	1.037-	5.995-
8	5.037-	2	2.332-	2	7.129-	3	2.016-	3	6.533-	3.099-	2.339-
9	1.126-	1	5.767-	2	1.064-	2	3.031-	3	2.027-	1.241-	7.723-
10	2.300-	2	1.078-	1	4.106-	2	1.439-	2	5.230-	3.361-	2.171-
11	1.079-	1	3.144-	3	4.576-	2	2.520-	2	1.155-	7.739-	5.190-
12	5.732-	1	1.060-	1	9.012-	2	4.715-	2	2.157-	462-	1.054-
13	6.562-	3	5.237-	1	1.374-	2	1.980-	2	2.534-	2.453-	1.702-
14	7.547-	2	2.791-	2	9.055-	2	3.751-	3	4.033-	2.075-	2.625-
15	6.441-	3	9.130-	2	3.390-	1	3.354-	2	1.123-	5.064-	1.237-
16	3.538-	3	2.113-	2	1.265-	1	3.251-	2	1.455-	9.704-	5.517-
17	1.754-	3	3.035-	3	7.591-	2	9.314-	2	1.716-	1.074-	4.153-
18	9.952-	0	5.152-	3	9.070-	2	2.112-	1	1.573-	1.500-	9.069-
19	2.394-	4	1.779-	4	9.033-	4	3.932-	3	1.715-	2.500-	0.253-
20	4.325-	5	3.014-	4	1.670-	2	1.640-	1	4.511-	1.070-	0.031-

Table 87

RKR FRANCK-CONDON FACTOR FOR (V2 PHOTO 4)

VV	0	1	2	3	4	5	6	7	8	9	10
V											
0	2.797-3	2.213-2	7.911-2	1.043-1	2.365-1	2.297-1	1.557-1	7.779-2	2.426-2	5.031-3	2.954-4
1	1.413-2	7.391-2	1.504-1	1.352-1	3.248-2	1.024-2	1.189-1	2.023-1	1.039-1	7.561-2	2.037-2
2	3.731-2	1.222-1	1.171-1	1.451-2	3.177-2	1.077-1	4.402-2	7.014-3	1.251-1	2.018-1	1.364-1
3	6.052-2	1.293-1	3.500-2	1.772-2	8.762-2	1.957-2	2.731-2	9.430-2	1.910-2	3.650-2	1.798-1
4	9.054-2	9.339-2	1.955-2	6.430-2	3.101-2	1.749-2	7.202-2	3.350-3	5.609-2	6.911-2	4.720-4
5	1.145-1	4.331-2	2.397-2	5.257-2	8.055-4	0.336-2	4.750-3	4.150-2	2.434-2	8.117-3	8.359-2
6	1.243-1	8.603-3	5.913-3	1.889-2	3.440-2	3.255-2	1.560-2	4.045-2	2.393-2	6.136-2	3.615-3
7	1.172-1	3.630-4	6.547-2	3.350-5	5.456-2	2.955-4	4.970-2	2.721-3	4.559-2	1.037-2	3.419-2
8	1.017-1	1.182-2	4.643-2	1.545-2	3.360-2	1.702-2	2.974-2	1.600-2	3.100-2	1.314-2	3.752-2
9	8.254-2	3.054-2	2.055-2	3.438-2	6.297-3	4.099-2	1.730-3	4.107-2	4.500-4	4.166-2	2.436-4
10	6.319-2	4.592-2	3.765-2	4.039-2	9.670-4	3.646-2	7.553-3	2.093-2	1.502-2	1.955-2	2.102-2

VV	11	12	13	14	15	16	17	18	19	20
V										
0	2.708-5	4.217-8	4.536-3	1.073-1	7.431-1	2.322-12	1.533-11	2.134-14	4.200-13	4.039-14
1	2.770-3	1.410-4	1.533-7	2.834-7	2.802-11	5.911-9	2.370-12	1.354-10	2.223-12	3.594-12
2	4.541-2	7.350-3	4.241-4	3.416-7	9.150-7	5.347-9	2.320-8	2.637-10	5.675-10	3.697-11
3	1.865-1	0.109-2	1.575-2	9.747-4	5.979-7	2.000-5	4.000-9	6.379-0	2.640-9	1.401-9
4	1.213-1	2.139-1	1.226-1	2.783-2	1.914-3	1.637-5	3.731-6	2.230-7	1.343-7	1.293-8
5	1.436-2	6.105-2	2.154-1	1.640-1	4.414-2	3.405-3	4.339-6	5.470-6	7.102-7	2.319-7
6	5.036-2	4.731-2	1.905-2	1.945-1	2.022-1	5.496-2	5.501-3	1.274-5	6.623-6	1.020-6
7	2.933-2	2.250-2	7.203-2	5.491-4	1.575-1	2.334-1	9.011-2	9.097-3	3.757-5	6.157-6
8	0.232-3	5.112-2	1.702-3	7.737-2	6.005-3	1.129-1	2.544-1	1.139-1	1.416-2	1.104-4
9	4.431-2	6.670-4	5.041-2	3.770-3	5.224-2	2.642-2	6.796-2	2.624-1	1.543-1	2.205-2
10	1.561-2	2.536-2	1.530-2	3.075-2	2.121-2	3.510-2	5.195-2	2.910-2	2.529-1	1.952-1

Table 88

RKR FRANK-CONDON FACTORS FOR (0,2) BANDS

V	V'	0	1	2	3	4	5	6	7	8	9	10	11
2-297-1	2-923-1	2-227-1	1-311-1	6-695-2	3-113-2	1-360-2	3-631-3	2-317-3	9-226-4	3-624-4	1-422-4		
3-899-1	4-771-2	2-491-2	1-100-1	1-460-1	1-150-1	7-425-2	4-120-2	2-109-2	1-015-2	4-679-3	2-436-3		
2-666-1	9-472-2	1-539-1	2-223-2	1-390-2	7-333-2	1-363-1	9-531-2	6-859-2	4-256-2	2-400-2	1-270-2		
3-398-2	2-907-1	5-630-5	1-194-1	9-006-2	7-041-3	1-459-2	5-012-2	9-439-2	7-993-2	6-070-2	4-031-2		
1-500-2	2-008-1	1-914-1	4-902-2	3-537-2	1-036-2	4-667-2	8-544-4	1-739-2	5-259-2	7-601-2	6-227-2		
5-1774-3	5-637-2	2-674-1	7-630-2	1-094-1	4-012-1	6-013-2	7-474-2	2-112-2	2-262-4	2-446-2	4-776-2		
6-7537-5	7-384-3	1-134-1	2-735-1	1-275-1	1-251-2	1-435-2	2-524-2	7-217-2	4-502-2	7-358-3	2-452-3		
7-1053-6	3-811-4	1-022-4	1-676-1	2-468-1	9-990-4	1-013-1	4-572-2	2-162-3	4-060-2	5-910-2	2-550-2		
8-2102-9	4-649-5	1-097-3	3-441-2	2-107-1	1-937-1	2-161-2	5-230-2	7-153-2	3-065-3	2-195-2	5-435-2		
9-6-26-9	1-413-3	1-153-5	2-322-3	3-514-2	2-593-1	1-359-1	5-334-2	2-717-2	7-055-2	1-057-2	4-510-3		
10-6-33-11	2-705-6	1-652-7	2-039-5	4-095-3	7-945-2	2-073-1	8-490-2	0-125-2	6-076-3	6-924-2	3-730-2		
11-5-774-10	1-971-3	4-257-4	8-590-7	2-927-5	6-397-3	1-061-1	3-032-1	4-590-2	9-792-2	9-776-6	3-119-2		
12-3-307-10	6-721-3	2-933-11	3-857-8	2-565-6	3-356-5	9-120-3	1-339-1	3-091-1	2-062-2	1-022-1	5-307-3		
13-6-271-11	3-200-11	1-032-8	2-636-9	3-908-8	6-226-6	2-040-5	1-231-2	1-630-1	3-004-1	6-225-3	9-694-2		
14-3-529-11	4-690-11	1-504-9	5-313-9	1-195-9	4-734-8	1-410-5	1-124-5	1-457-2	1-060-1	3-047-1	7-453-4		

Table 88 (cont'd)

(12) 2010 11

V	12	13	14	15	16	17	18	19	20	21	22	23											
5	5.595-	5	2.219-	5	3.308-	6	3.532-	6	1.377-	6	5.159-	7	1.856-	7	5.515-	8	2.424-	3	1.113-	3	7.119-	3	5.090-
1	9.166-	4	3.938-	4	1.077-	4	7.122-	5	3.030-	5	1.239-	5	5.025-	6	2.457-	6	1.104-	6	5.122-	7	2.517-	7	1.332-
2	0.397-	3	3.106-	3	1.471-	3	5.052-	4	3.151-	4	1.458-	4	5.774-	5	3.131-	5	1.531-	5	7.527-	6	3.705-	6	1.930-
3	2.434-	2	1.378-	2	7.437-	3	3.079-	3	1.975-	3	9.325-	4	4.959-	4	2.434-	4	1.249-	4	6.376-	5	3.294-	5	1.705-
4	5.320-	2	3.699-	2	2.349-	2	1.400-	3	0.056-	3	4.400-	3	2.442-	3	1.315-	3	7.030-	4	3.771-	4	2.021-	4	1.073-
5	0.069-	2	5.701-	2	4.045-	2	3.330-	2	2.210-	2	1.396-	2	0.454-	3	4.990-	3	2.077-	3	1.643-	3	9.279-	4	5.130-
6	2.290-	2	4.353-	2	5.270-	2	4.990-	2	4.075-	2	3.417-	2	2.105-	2	1.375-	2	9.714-	3	5.393-	3	3.259-	3	1.936-
7	1.422-	3	5.026-	3	2.410-	2	4.004-	2	4.606-	2	4.333-	2	3.000-	2	2.739-	2	1.958-	2	1.340-	2	0.023-	3	5.541-
8	4.144-	2	1.199-	2	3.336-	7	0.500-	3	2.434-	2	3.625-	2	4.430-	2	3.790-	2	3.197-	2	2.494-	2	1.029-	2	1.257-
9	3.046-	2	4.747-	2	2.501-	2	4.579-	3	7.037-	4	1.051-	2	2.353-	2	3.254-	2	3.542-	2	3.339-	2	2.060-	2	2.134-
10	1.167-	4	2.016-	2	4.236-	2	3.596-	2	1.464-	2	1.223-	3	2.034-	3	1.153-	2	2.205-	2	2.097-	2	3.094-	2	2.029-
11	5.057-	2	0.191-	3	5.412-	3	3.149-	2	3.009-	2	2.432-	2	7.080-	3	1.212-	4	3.213-	3	1.172-	2	2.009-	2	2.451-
12	3.136-	2	5.447-	2	1.751-	2	3.192-	4	1.016-	2	3.474-	2	3.147-	2	1.640-	2	3.000-	3	3.154-	5	3.957-	3	1.071-
13	1.092-	2	1.436-	2	5.102-	2	2.087-	2	1.549-	3	7.307-	3	2.604-	2	2.252-	2	2.411-	2	1.073-	2	1.776-	3	2.330-
14	8.504-	2	3.015-	2	4.553-	3	4.123-	2	3.652-	2	7.696-	3	1.202-	3	1.535-	2	2.092-	2	2.033-	2	1.001-	2	6.059-

Table 89

RKR FRANCK-CONDON FACTORS FOR (3/2) P(3/2 2)

V	V'	0	1	2	3	4	5	6	7	8	9	10	11
0	9.841-3	5.379-2	1.372-1	2.139-1	1	2.286-1	1.789-1	1.059-1	4.037-1	1.724-2	4.886-2	3	2.034-4
1	3.586-2	1.226-1	1.575-1	7.425-2	2	7.309-4	5.057-2	1.493-2	1.794-1	1.303-1	6.637-2	2	7.159-3
2	7.159-2	1.406-1	5.138-2	1.966-3	3	8.123-2	9.004-2	1.478-2	2.111-2	1.103-1	1.567-1	1	6.330-2
3	1.040-1	1.023-1	1.517-3	6.166-2	4	7.093-2	4.403-4	5.097-2	0.917-2	1.445-2	2.192-2	2	1.637-1
4	1.234-1	4.672-2	1.072-2	7.731-2	5	3.973-3	4.005-2	5.324-2	7.683-8	6.313-2	7.641-2	3	3.023-2
5	1.272-1	9.153-3	5.664-2	3.237-2	6	1.081-2	6.155-2	3.320-4	5.626-2	4.189-2	4.117-3	2	5.474-2
6	1.102-1	3.220-4	5.050-2	1.131-3	7	5.404-2	1.324-2	3.202-2	4.301-2	3.797-3	6.404-2	2	2.254-2
7	1.016-1	1.237-2	5.120-2	9.040-2	8	4.770-2	3.150-3	5.247-2	4.120-4	5.000-2	1.760-2	2	5.944-2
8	8.226-2	3.205-2	2.434-2	3.460-2	9	1.671-2	3.031-2	2.372-2	2.242-2	3.376-2	8.263-3	2	3.734-4
9	6.357-2	4.922-2	5.209-3	4.021-2	10	2.240-4	4.459-2	2.300-3	4.394-2	7.707-4	4.333-2	3	3.473-2
10	4.726-2	5.098-2	6.008-5	4.316-2	11	7.522-3	5.033-2	1.339-2	2.575-2	1.444-2	2.969-2	2	3.791-2

V	V'	12	13	14	15	16	17	18	19	20	21	22	23
0	2.909-5	2.015-5	1.947-7	3.215-6	7.302-9	9.432-10	2.315-9	1.757-9	1.370-9	5.489-10	1.529-9	7.003-13	9.581-13
1	1.563-3	2.571-4	3.179-5	3.459-6	3.256-7	3.256-7	2.315-9	1.022-9	2.056-9	1.359-9	2.380-9	1.701-10	1.000-9
2	2.378-2	5.347-3	1.203-3	1.037-4	2.045-5	2.045-5	1.635-6	7.055-8	4.200-9	1.356-9	3.722-10	5.214-10	9.373-10
3	1.165-1	5.492-2	1.031-2	4.220-3	7.204-4	7.204-4	9.050-5	0.404-6	4.641-7	1.054-8	1.400-9	3.247-10	1.329-10
4	1.350-1	1.532-1	3.660-2	3.944-2	1.112-2	1.112-2	2.214-3	3.135-4	3.034-5	1.909-6	9.752-6	2.576-6	5.465-3
5	0.553-5	7.002-2	1.524-2	1.363-1	7.109-2	7.109-2	2.410-2	5.591-3	0.931-4	9.991-5	0.241-6	7.942-7	1.728-7
6	8.310-2	2.493-2	1.351-2	1.121-1	1.576-1	1.576-1	1.002-1	4.487-2	1.215-2	2.243-3	2.908-4	3.374-5	4.050-5
7	7.211-4	5.420-2	6.041-2	1.064-3	5.392-2	5.392-2	1.490-1	1.447-1	7.296-2	2.340-2	5.121-3	0.491-4	1.230-4
8	5.091-2	3.084-2	1.032-2	7.073-2	3.100-2	3.100-2	9.985-3	1.110-1	1.530-1	1.049-1	4.101-2	1.046-2	2.334-3
9	2.771-2	1.215-2	5.000-2	2.707-3	4.709-2	4.709-2	6.051-2	1.577-3	5.096-2	1.520-1	1.342-1	6.632-2	2.242-2
10	2.636-3	4.907-2	1.036-3	4.515-2	3.152-2	3.152-2	1.010-2	7.039-2	2.590-2	1.590-2	1.179-1	1.542-1	1.024-1

Table 90

RKR FRANK-CONDON FACTORS FOR (312) PHOTO 31

V	0	1	2	3	4	5	6	7	8	9	10	11									
2.355-	3	1.975-	2	1.290-	1	1.051-	1	2.037-	1	1.705-	1	1.154-	1	6.472-	2	3.003-	2	1.101-	2	3.919-	3
1.303-	2	5.123-	2	1.307-	1	6.245-	2	3.026-	3	2.441-	2	9.970-	2	1.500-	1	1.433-	1	9.942-	2	5.327-	2
3.137-	2	3.941-	2	3.594-	2	2.525-	3	6.251-	2	9.192-	2	3.710-	2	1.632-	4	4.633-	2	1.102-	1	1.410-	1
5.474-	2	1.135-	1	5.511-	4	5.604-	2	6.590-	2	5.142-	3	2.427-	2	0.005-	2	5.427-	2	2.503-	3	2.651-	2
7.762-	2	9.156-	2	3.253-	2	0.314-	2	5.019-	3	2.767-	2	5.491-	2	1.495-	2	1.212-	2	6.901-	2	5.794-	2
9.507-	2	5.691-	2	5.912-	3	2.011-	2	1.320-	2	5.625-	2	1.040-	2	1.009-	2	5.907-	2	1.072-	2	9.055-	3
1.344-	1	2.417-	2	4.024-	2	4.043-	5	4.522-	2	2.078-	2	1.336-	2	5.009-	2	9.557-	3	1.049-	2	5.013-	2
1.052-	1	4.439-	3	1.966-	2	1.662-	2	3.359-	4	1.353-	4	4.141-	2	1.602-	2	1.216-	2	4.600-	2	5.051-	3
9.910-	2	2.710-	4	1.520-	3	3.700-	2	1.222-	2	1.004-	2	3.133-	2	1.519-	3	4.049-	2	9.206-	3	1.790-	2
4.310-	2	7.750-	3	3.101-	3	3.031-	2	3.056-	6	3.545-	2	4.051-	3	2.469-	2	2.107-	2	5.796-	3	3.450-	2
7.409-	2	2.334-	2	1.607-	2	2.278-	2	9.557-	3	2.737-	2	2.530-	3	3.292-	2	4.126-	4	3.015-	2	1.154-	2

V	12	13	14	15	16	17	18	19	20	21	22	23								
1	1.092-	3	2.549-	5	9.401-	6	1.243-	7	4.724-	9	7.036-	9	2.007-	9	2.590-	9	2.570-11	11	2.045-	9
1	2.205-	2	0.027-	3	5.673-	4	1.919-	5	2.520-	6	3.612-	7	4.279-	6	2.610-10	10	1.031-14	14	2.430-	9
2	1.110-	1	0.539-	2	1.052-	3	7.021-	4	1.473-	4	2.357-	5	3.137-	5	3.932-	7	5.429-	9	1.232-	9
3	9.919-	2	1.304-	1	6.062-	2	1.116-	2	3.195-	3	7.362-	4	1.304-	4	2.295-	5	3.949-	6	7.153-	7
4	4.796-	3	2.116-	2	1.328-	1	6.532-	2	2.967-	2	1.021-	2	2.007-	3	6.413-	4	1.347-	4	2.033-	5
5	0.552-	2	5.524-	2	2.313-	2	1.310-	1	1.475-	1	5.000-	2	2.500-	2	0.634-	3	2.404-	3	6.543-	4
6	1.346-	2	1.229-	2	4.000-	2	3.072-	2	1.020-	1	1.231-	1	9.003-	2	5.204-	2	2.229-	2	0.151-	3
7	2.290-	2	5.233-	2	6.759-	2	3.070-	2	0.042-	7	4.256-	2	1.095-	1	1.220-	1	0.051-	2	4.992-	2
8	4.191-	2	1.565-	3	4.629-	3	2.921-	2	6.034-	2	2.679-	2	1.709-	3	5.450-	2	1.140-	1	1.251-	1
9	3.042-	3	2.579-	2	4.302-	2	3.654-	2	1.005-	5	4.241-	2	6.414-	2	1.542-	2	7.407-	3	7.727-	2
10	1.330-	2	3.323-	2	3.402-	2	3.535-	3	4.675-	2	2.433-	2	3.211-	3	5.272-	2	5.335-	2	4.391-	3

Table 91

RKR FRANCK-CONDON FACTORS FOR (312) π W(12) π

V	VV	0	1	2	3	4	5	6	7	8	9	10	11
1	4.120-1	3.731-1	1.612-1	4.376-2	0.423-3	1.246-3	1.246-3	1.500-4	1.436-5	9.134-7	6.000-8	9.904-9	5.466-10
2	3.373-1	2.865-1	2.316-1	2.605-1	1.233-1	3.596-2	3.596-2	7.304-3	1.126-3	1.335-4	1.219-5	1.162-5	1.179-7
3	1.620-1	1.714-1	0.140-2	4.749-2	2.204-1	1.350-1	1.350-1	0.476-2	2.344-2	4.644-3	7.057-4	0.514-5	9.380-6
4	6.059-2	2.117-1	1.790-2	1.611-1	2.002-3	1.157-1	1.157-1	2.150-1	1.426-1	5.383-2	1.307-2	2.607-3	3.391-4
5	1.973-2	1.304-1	1.324-1	1.509-2	1.106-1	6.439-2	6.439-2	2.149-2	1.686-1	1.030-1	9.734-2	3.204-2	7.989-3
6	5.938-3	6.476-2	1.537-1	3.308-2	0.252-2	3.233-2	3.233-2	1.208-1	3.292-3	0.342-2	1.446-1	1.432-1	0.333-2
7	1.700-3	2.646-2	1.117-1	1.141-1	4.952-4	1.439-1	1.439-1	4.109-4	1.053-1	4.974-2	1.496-2	1.303-1	1.712-1
8	4.770-4	9.442-3	0.002-2	1.203-2	4.241-2	3.029-2	3.029-2	5.927-2	3.573-2	4.332-2	9.795-2	3.604-3	6.079-2
9	1.294-4	3.142-3	2.739-2	3.441-2	1.004-1	1.457-3	1.457-3	7.007-2	1.332-2	0.193-2	1.505-3	9.504-2	4.151-2
10	3.332-5	1.011-3	1.120-2	5.479-2	1.003-1	4.559-2	4.559-2	1.453-2	7.541-2	2.035-3	7.030-2	1.631-2	4.742-2
11	7.705-6	3.022-4	4.207-3	2.732-2	0.200-2	0.737-2	0.737-2	5.020-3	5.230-2	3.203-2	3.767-2	3.203-2	5.094-2

III

V	VV	12	13	14	15	16	17	18	19	20	21	22	23
1	1.726-10	2.077-12	3.903-11	6.640-11	1.025-11	1.025-11	2.554-11	9.725-11	1.796-11	2.419-11	6.313-11	9.403-12	7.437-12
2	3.402-9	2.620-11	1.032-10	2.521-10	1.263-10	1.263-10	9.332-11	5.221-11	4.070-11	7.143-11	1.146-10	9.734-12	1.930-10
3	0.076-7	9.307-9	1.139-10	3.936-9	1.012-9	1.012-9	1.122-9	0.504-10	1.111-9	1.105-10	9.493-10	3.430-11	2.041-10
4	4.717-5	3.934-8	1.705-7	4.308-8	1.631-8	1.631-8	3.033-9	2.500-9	2.557-9	6.609-10	1.310-9	3.134-11	1.443-9
5	1.403-3	1.938-6	2.121-5	1.093-5	1.907-6	1.907-6	6.010-7	2.949-9	1.312-9	2.492-9	2.009-9	3.127-10	1.453-9
6	1.902-2	4.160-3	6.976-4	9.131-5	9.025-6	9.025-6	0.037-7	5.461-8	1.119-9	9.104-10	5.990-11	1.208-9	7.753-10
7	1.027-1	3.937-2	1.057-2	2.107-3	3.240-4	3.240-4	3.094-5	4.090-6	2.090-7	7.603-9	1.477-9	1.725-9	1.010-11
8	1.644-1	1.411-1	6.981-2	2.316-2	5.506-3	5.506-3	1.427-3	1.448-4	1.649-5	1.310-5	1.103-7	3.442-8	1.205-9
9	1.123-2	1.193-1	1.014-1	1.060-1	4.404-2	4.404-2	1.309-2	2.051-3	4.095-4	6.322-5	7.330-6	1.172-6	3.110-7
10	0.461-2	3.323-3	5.530-2	1.493-1	1.403-1	1.403-1	7.543-2	2.712-2	7.093-3	1.415-3	2.422-4	4.105-5	0.924-6
11	4.514-3	0.621-2	3.907-2	7.000-3	1.035-1	1.035-1	1.546-1	1.112-1	5.020-2	1.623-2	4.074-3	9.277-4	2.192-4

Table 92

K_K FRANK-CONDON FACTORS FOR (312) PHOTO 51

V	0	1	2	3	4	5	6	7	8	9	10	11
0	6.750-2	1.538-1	2.110-1	2.073-1	1.639-1	1.024-1	5.513-2	2.552-2	1.033-2	3.728-3	1.213-3	3.443-4
1	1.943-1	1.691-1	5.057-2	1.542-2	4.226-2	1.136-1	1.112-1	1.251-1	0.336-2	4.566-2	2.129-2	4.443-3
2	2.538-1	4.170-2	1.208-2	9.076-2	0.091-2	1.578-2	5.675-3	5.240-2	1.149-1	1.225-1	9.402-1	5.725-2
3	2.299-1	9.952-3	9.944-2	4.060-2	1.122-3	5.223-2	7.045-2	2.734-2	4.640-4	3.314-2	9.566-2	1.152-1
4	1.522-1	9.858-2	5.323-2	2.092-3	6.699-2	4.240-2	2.412-6	4.140-2	7.093-2	3.220-2	2.300-3	2.944-2
5	7.592-2	1.798-1	7.360-5	5.151-2	3.956-2	4.174-3	5.302-2	3.073-2	5.534-7	3.537-2	6.577-2	3.155-2
6	2.777-2	1.734-1	5.151-2	4.249-2	2.632-4	5.053-2	2.144-2	5.272-3	5.147-2	3.150-2	4.208-5	3.517-2
7	6.509-3	1.146-1	1.413-1	0.433-4	3.096-2	3.411-2	7.044-3	4.555-2	1.524-2	9.663-3	4.015-2	2.559-2
8	5.903-4	4.733-2	1.630-1	3.533-2	2.958-2	3.762-5	5.119-2	1.059-2	1.155-2	4.520-2	6.055-3	1.373-2
9	5.144-5	1.222-2	1.229-1	1.109-1	7.753-4	1.753-2	3.203-2	1.077-2	3.554-2	5.069-3	2.102-2	3.020-2
10	3.901-4	9.251-4	5.433-2	1.577-2	2.039-2	1.940-2	0.511-4	6.750-2	5.091-3	1.391-2	3.540-2	1.511-4

V	12	13	14	15	16	17	18	19	20	21	22	23
0	0.760-5	1.009-3	3.744-3	7.019-7	1.427-7	0.254-9	1.423-13	2.290-9	3.470-10	9.595-14	1.022-11	4.908-13
1	2.903-3	0.643-4	2.251-4	5.307-5	1.125-5	1.745-6	2.393-7	5.341-6	9.703-9	7.302-13	1.172-12	2.220-9
2	2.036-2	1.102-2	4.130-2	1.280-3	3.424-4	7.019-5	1.532-5	2.774-6	4.429-7	4.119-8	5.905-9	6.137-9
3	9.720-2	0.244-2	3.249-2	1.302-2	4.007-3	1.531-3	3.934-4	0.707-5	1.682-5	3.023-6	5.310-7	1.130-7
4	9.477-2	1.114-1	9.712-2	5.332-2	3.297-2	1.430-2	4.968-3	1.476-3	3.730-4	0.400-5	1.002-5	4.231-6
5	1.105-4	2.701-2	0.119-2	1.003-1	3.473-2	6.157-2	3.146-2	1.314-2	4.434-3	1.334-3	3.559-4	9.451-5
6	6.148-2	2.042-2	3.557-2	2.093-2	0.252-2	1.070-1	9.095-2	5.717-2	2.025-2	1.147-2	4.090-3	1.379-3
7	0.516-4	3.740-2	5.446-2	2.311-2	2.986-4	3.455-2	0.673-2	1.054-1	0.453-2	5.113-2	2.545-2	1.134-2
8	4.729-2	1.027-2	2.406-3	4.210-2	5.449-2	1.650-2	2.033-3	4.247-2	0.900-2	9.905-2	7.360-2	5.075-2
9	2.507-3	2.056-2	4.336-2	1.101-2	6.503-3	4.745-2	4.937-2	1.031-2	5.522-3	4.936-2	9.256-2	1.051-1
10	2.594-2	3.006-2	9.533-5	2.660-2	4.015-2	5.231-3	1.291-2	5.252-2	4.224-2	4.934-3	1.100-2	6.544-2

Table 93 RKR FRANCK-CONDON FACTORS FOR (312) 3412 61

v	v'	2	3	4	5	6	7	8	9	10	11
0	4.722-1	1.212-1	4.845-3	1.554-3	3.397-5	5.298-5	3.993-5	2.550-6	1.505-6	2.343-6	2.112-7
1	3.409-2	5.623-1	1.642-3	1.148-2	5.918-3	4.442-4	5.717-5	1.456-4	4.314-5	7.277-7	2.773-5
2	3.234-2	1.336-1	3.106-1	4.879-3	2.041-2	1.446-2	1.730-3	6.015-5	3.971-4	1.804-4	2.111-5
3	3.708-4	7.724-2	1.479-1	3.691-1	1.249-2	2.323-2	2.810-2	4.504-3	4.493-5	9.074-4	5.716-4
4	3.295-4	3.754-3	1.323-1	2.130-1	3.929-1	2.321-2	3.544-2	4.524-2	9.330-3	1.577-5	1.757-3
5	2.337-6	1.703-3	1.913-1	1.148-1	1.272-1	3.097-1	3.635-2	4.083-2	6.761-2	1.606-2	1.722-5
6	7.696-6	6.504-3	1.279-2	2.447-1	8.720-2	5.635-2	3.621-1	5.000-2	4.226-2	9.014-2	2.729-2
7	5.316-6	6.124-3	1.031-2	1.818-2	2.318-1	5.195-2	2.742-2	3.172-1	6.176-2	4.674-2	1.117-1
8	3.715-6	2.476-5	6.517-5	1.966-2	2.451-2	3.254-1	3.824-2	6.045-3	2.615-1	7.072-2	3.695-2
9	1.227-5	1.014-5	6.542-4	1.594-4	3.143-2	3.120-2	3.470-1	2.123-2	4.145-2	2.006-1	7.044-2
10	2.754-7	3.008-5	2.355-5	1.447-3	2.951-4	4.295-2	3.876-2	3.590-1	1.894-2	2.603-3	1.417-1

v	v'	12	13	14	15	16	17	18	19	20	21	22	23											
0	2.491-	7	5.636-	7	1.919-	7	5.710-10	1.014-	7	1.236-	7	4.225-	4	7.730-10	1.170-	4	2.457-	8	1.746-	4	4.924-	9		
1	2.175-	6	7.772-	4	3.544-	7	5.167-	7	9.235-	8	4.193-	6	2.374-	7	2.134-	7	5.210-	7	2.530-	9	5.858-	8	8.300-	9
2	3.475-	7	5.949-	6	2.534-	6	3.703-	8	2.017-	7	2.559-	7	2.455-	4	5.257-	8	1.740-	7	1.306-	7	2.192-	8	7.248-	9
3	1.346-	4	9.559-	4	1.341-	5	1.228-	5	3.125-	6	3.480-	6	3.206-	7	3.122-	7	2.976-	7	4.776-	4	1.607-	7	1.154-	7
4	1.348-	3	3.109-	4	5.230-	6	2.291-	5	3.340-	5	1.449-	5	1.974-	5	3.740-	8	5.801-	7	3.635-	7	2.443-	4	4.039-	4
5	2.995-	3	2.770-	3	9.080-	4	3.813-	5	3.354-	5	7.597-	5	4.555-	5	1.170-	5	5.121-	7	5.207-	7	1.099-	6	5.172-	7
6	3.200-	5	4.635-	3	5.132-	3	1.753-	3	1.318-	4	4.403-	3	1.547-	4	1.155-	4	4.022-	5	4.334-	6	1.527-	7	1.491-	5
7	4.110-	2	3.676-	4	5.575-	3	8.533-	3	3.378-	3	3.499-	4	4.905-	4	2.822-	4	2.533-	4	1.886-	4	2.523-	5	1.401-	7
8	1.302-	1	3.407-	2	1.008-	3	8.610-	3	1.318-	2	5.978-	3	7.408-	4	4.475-	5	4.742-	4	5.801-	4	2.496-	4	6.153-	5
9	3.132-	2	1.436-	1	7.036-	1	2.121-	3	1.045-	2	1.691-	2	9.793-	3	1.536-	3	2.990-	3	7.462-	4	9.017-	4	4.975-	4
10	7.694-	2	2.426-	2	1.511-	1	8.482-	2	3.746-	3	1.131-	2	2.525-	2	1.490-	2	2.944-	3	5.265-	6	1.000-	3	1.474-	3

Table 94

TABLE OF FRANCK-CONDON FACTORS BY VARIOUS INVESTIGATORS

<u>Molecule</u>	<u>System</u>	<u>Reference</u>
CN	Red (A-X)	33
CN	Violet (B-X)	33
CO	4(+) (A-X)	33
CO ⁺	Comet tail (A-X)	34
CO ⁺	(1-) (B-X)	34
N ₂	(1+) (B-A)	33, 35, 36, 37, 29
N ₂	(2+) (C-B)	33, 35, 36, 37
N ₂	Vegard Kaylan (A-X)	35, 37, 29
N ₂	y bands (B'-B)	36
N ₂	y bands (a-a')	36
N ₂	y bands (w-a)	36
N ₂	LBH (a-x)	37
N ₂	Tanaka (c-x)	37
N ₂	B-H (b', b-x)	33
N ₂ ⁺	Meinel (A-X)	33
N ₂ ⁺	(1-) (B-X)	33
N ₂ ⁺	(2-) (C-X)	33
NO	B (A-X)	33, 38
NO	γ (B-X)	33, 38
NO	δ (C-X)	33
NO	ε (D-X)	33
NO	β' (B'-X)	33
NO	γ' (E-X)	33

Table 94 (cont'd)

<u>Molecule</u>	<u>System</u>	<u>Reference</u>
NO	Lagerquist-Miescher (G-X)	33
NO	Heath (C-A)	
NO	Feast 1 (D-A)	33
NO	Feast 2 (E-A)	33
	Feast 2 (E-C)	33
NO	Feast-Heath (E-D)	33
O ₂	Schumann-Runge (B-X)	33, 39

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APPENDIX I

COMPUTER PROGRAM TURNGPT

A listing of the computer program used to generate the RK potentials at AFWL is included in this appendix. The input data needed is described and a sample data deck is also included.

1. INPUT DATA

The reduced mass of the molecule or the mass at each atom is needed. These can be based on either C_{12} or O_{16} . A good source for reduced masses based on O_{16} is Herzberg (Ref. 31).

The energy levels of the molecule can be constructed internally in the program if the spectroscopic constants w_e , w_{ex} , w_{ey} , w_{ez} , w_{exy} are read in. These are used in the equation.

$$E = w_e(v+1/2) - w_{ex}(v+1/2)^2 + w_{ey}(v+1/2)^3 \\ + w_{ez}(v+1/2)^4 + w_{exy}(v+1/2)^5 + \dots$$

Herzberg (Ref. 31) has a large tabulation of these. Alternatively, one can use the G_v obtained from spectroscopic data. Wallace (Refs. 24, 40) has an extensive tabulation of these.

One also needs the relational constants, that is, either B_e , α_e , δ_e , γ_e , ϵ_e , or the B_v for the various vibrational levels. Again Herzberg (Ref. 31) is a good source for B_e , α_e , γ_e and Wallace (Refs. 24, 40) is a good source for the B_v . The final bit of data about the molecule that is needed is the equilibrium internuclear separation. This can be found in Herzberg (Ref. 31).

2. DATA DECK

The data deck set-up procedure needs very little explanation since Zare has made extensive use of comment cards throughout his program.

Card Number

1	ITEST I1	1 if problem follows
2, 3	FMT 8A10	Title of the problem with carriage control in column 1
4	IIMS, ZMAS1, ZMAS2 IF, 2E10.0	IIMS = 1 mass based on C = 12 IIMS = 2 mass based on O = 16 ZMAS1 mass of first atom (or reduced mass of molecule) ZMAS2 mass of second atom (or blank when using reduced mass)
5	IQHK, N 2I4, 4x, 6A10	IQHK = 0 using a tabulated Gv curve. Format for Gv in columns 13-72. IQHK \neq 0 using constants to generate Gv curve. Hollerith text in columns 13-72. N - number of vibrational levels to be used
6a	WE, WEXE, WEYE, WEZE, WETE, 5E10.0	Use when IQHK \neq 0. These are the spectroscopic constants that generate the energies of the vibrational levels.
6b	G(I) Format in columns 13-72 of Card 5	Use when IQHK = 0. These are the Gv of spectroscopy.
7	IOPEV I1	IOPEV = 0 if zero point energy to be found by extrapolation IOPEV = 1 tabulated Gv curve to be used unchanged IOPEV = 2 if Gv curve is to be constructed from constants
8	IBHK, N 2I4, 4x	IBHK = 0 using tabulated Bv curve. Format for Bv in columns 13-72.

Card Number

Card 8 (cont'd)

		IBHK \neq 0 constants are used to generate Bv curve. Hollerith text in columns 13-72.
		N - number at vibrational levels (same as above)
9a	BE, ALPHA E, GAMMA E, DELTA E, 5E10.0	Use when IBHK \neq 0; these were used to generate the Bv
9b	B(v) Format in columns 13-72 of Card 8	Use when IBHK = 0
10	IOPA, BEQUIL I4, 3F10.0	IOPA = 0 value of BE to be found by extrapolation from Bv data read in IOPA = 1 value of BE given by BEQUIL IOPA = 2 rotational constants are used (leave BEQUIL blank) BEQUIL - spectroscopic constant Be
11	RE F10.0	Internuclear equilibrium distance
12	VSTART, VFIN, HDED 3E10.0	Turning points are calculated from vibrational level VSTART to VFIN to steps of HDED
13	IOPFG I1	IOPFG = 0 intermediate printout skipped IOPFG = 1 intermediate steps in an evaluation of the Klein integrals are to be printed out
14	Blank	

```

PROGRAM TURNPT(INPUT,OUTPUT,TAPES=INPUT,TAPE6=OUTPUT,FILMPL,PUNCH A 1
1,TAPE7=PUNCH) A 2
C SET-UP FOR PLOTTING POTENTIALS... A 3
CALL INIT280 A 4
C MAIN FINDS TURNING POINTS FOR A MOLECULE BY HYDBERG-KLEIN-REES MET A 6
C ALL INPUT IS IN WAVE NUMBERS AND ANGSTROMS. A 7
C USER SPECIFIES CHOICE BETWEEN MASS UNITS BASED ON C12 = 12, OR A 8
C O16 = 16. A 9
C THE FOLLOWING COMMENT CARDS DESCRIBE THE PREPARATION OF DATA CARDS A 10
C
DIMENSION VSTART(1), VFIN(1), HDEF(1) A 11
DIMENSION XI(200), YI(200), XO(3000), V(3000), S(3000), XV(200), F A 12
ITRIAL(200), QIPA(2), QIFN(3), QIMS(2), ZIMS(2), ZIPA(2), ZIFN(2), A 13
2FCALC(200), XORN(5), VORN(5), DIERMT(6), G(200), RV(200), FMT(16), A 14
3 U(200), RMIN(200), RMAX(200), DUFMT(6), RVF(200), GI(200), RVI(20 A 15
40), J(20), DV(30), RVF(30), DVE1(30), DVE2(30), A(30), Y(30), XX(6 A 16
5), YY(6), ANS(3), XNN(5), XFL(1), XFE(1), FL(1), D3(2), GB(30), YY A 17
6Y(6), SIGH(1) A 18
COMMON XI,YI,XO,V,XH,NSTA,N,MSTA,M,XMIN,XMAX,INSC,MREG,NUSED,S,NI, A 19
INS,MAXIT,FACM,ZMU,DE,WE,WEXE,WEYE,WEZE,WETE,DE,ALPHA, GAMMA,DELTA A 20
2F,AS,BS,MO,STEP,U,PV,C,ICK,H,ITR,HDES,EP,SLNE,XY,REQUIL,ZPTEN,MLV,L A 21
DV,RE,VSTART,VFIN,HDEF A 22
REAL J1,J2,J3,J4,JHAF2 A 23
C FIRST CARD IN DATA HAS A ONE IN COLUMN 1 IF A PROBLEM FOLLOWS. A 24
C VERY LAST CARD IN DATA MUST BE A BLANK CARD..... A 25
C A 26
C A 27
1 CONTINUE A 28
READ (5,50) ITEST A 29
IF (ITEST) 2,40,2 A 30
C A 31
C NEXT TWO CARDS IN DATA HAVE NAME OF PROBLEM IN COLUMNS 1-80. A 32
C WHERE CARRIAGE CONTROL IS IN COLUMN 1. NEXT CARD HAS IIMS AND A 33
C MASSES OF THE TWO ATOMS, OR IIMS AND REDUCED MASS IN FIRST MASS A 34
C FIELD WITH SECOND BLANK. A 35
C IIMS = 1. MASS UNITS ARE BASED ON C12 = 12. A 36
C IIMS = 2. MASS UNITS ARE BASED ON O16 = 16. A 37
C A 38
2 READ (5,51) (FMT(I),I=1,16) A 39
READ (5,52) IIMS,ZMAS1,ZMAS2 A 40
C A 41
C NEXT CARD IN DATA HAS IQHK, AND NUMBER OF LEVELS, EACH A 42
C IN 14 FORMAT, AS WELL AS THE FORMAT STATEMENT WHICH CONTROLS THE A 43
C READING OF THE LEVELS (IN COLUMNS 13-72)--FOR EXAMPLE- (4F16.8). A 44
C IQHK = 0 IF THE FOLLOWING CARDS CONTAIN THE TABULATED G CURVE. A 45
C IF A PARTICULAR VALUE IS TO BE INTERPOLATED, SET G(I) = -10. A 46
C IF IT IS DESIRED TO USE CONSTANTS TO GENERATE THE ENTIRE A 47
C G CURVE, IQHK MUST NOT BE EQUAL TO ZERO. A 48
C A HOLLERITH TEXT MUST BE PUNCHED IN COLUMNS 12-72. A 49
C AS IT WILL BE PRINTED, E.G., (1H ) A 50
C THE NEXT CARD IN SUCH A CASE CONTAINS A 51
C WE,WEXE,WEYE,WEZE,AND WETE. A 52
C A 53
READ (5,53) IQHK,N,(DIERMT(I),I=1,6) A 54
IIFN=2 A 55

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	IF (IQHK) 3,4,2	A 54
3	READ (5,54) WF,WEXF,WEYF,WEZF,WETF	A 55
	GO TO 5	A 56
4	READ (5,DTERMT) (GI(I),I=1,N)	A 57
C		A 58
C	THE ZERO POINT ENERGY MAY BE FOUND BY EXTRAPOLATION, OR IT MAY BE	A 59
C	FIXED BY THE USER FROM HIS TABULATED G(V) CURVE.	A 60
C	NEXT CARD CONTAINS IOPEV.	A 61
C	SET IOPEV = 0, IF THE ZERO POINT ENERGY IS TO BE FOUND BY	A 62
C	EXTRAPOLATION, AND THE G(V) CURVE IS TO BE RAISED OR LOWERED	A 63
C	ACCORDINGLY.	A 64
C	THIS IS PARTICULARLY USEFUL IF DELTA G(V) DATA IS TO BE USED.	A 65
C	SET IOPEV = 1, IF THE TABULATED G(V) CURVE IS TO BE USED UNCHANGED	A 66
C	SET IOPEV = 2, IF THE G(V) CURVE IS TO BE CONSTRUCTED FROM CONSTAN	A 67
C		A 68
5	READ (5,50) IOPEV	A 69
C		A 70
C	THE NEXT SET OF CARDS CONTAINS THE RV CURVE WITH THE SAME	A 71
C	RESTRICTIONS AS FOR G CURVE ABOVE. NUMBER OF VALUES HERE MUST BE	A 72
C	EQUAL TO THE NUMBER ABOVE	A 73
C		A 74
	READ (5,53) IRHK,N,(DUENT(I),I=1,6)	A 75
	IIEB=2	A 76
	IF (IRHK) 6,7,6	A 77
6	READ (5,54) BE,ALPHA, GAMMA, DELTA, EPSLN	A 78
	GO TO 8	A 79
7	READ (5,DUENT) (RVI(I),I=1,N)	A 80
C		A 81
C	THE ROTATIONAL CONSTANT BE MAY BE FOUND BY EXTRAPOLATION, OR IT	A 82
C	MAY BE FIXED BY THE USER.	A 83
C	NEXT CARD CONTAINS IOPA AND REQUIL.	A 84
C	SET IOPA = 0, IF THE VALUE OF BE IS TO BE FOUND BY EXTRAPOLATION	A 85
C	FROM THE RV DATA READ IN. LEAVE REQUIL BLANK.	A 86
C	SET IOPA = 1, IF THE VALUE OF BE IS TO BE GIVEN BY REQUIL.	A 87
C	SET IOPA = 2, IF ROTATIONAL CONSTANTS ARE USED. LEAVE REQUIL	A 88
C	BLANK.	A 89
C		A 90
8	READ (5,52) IOPA,REQUIL	A 91
C		A 92
C	READ IN HIGHER TERMS IN EXPANSION RV,HV,COUPLING CONSTANT A,LAMDA,	A 93
C	GAMMA OFA MULLIKEN FORMULA,NUMBER OF J LEVELS TO BE CALCULATED NJ,	A 94
C	AND IND (=1 2 3) TO INDICATE EXPANSION FORM 1 FOR SINGLET SIGMA	A 95
C	2 FOR DOUBLET P1 1/2 3 FOR DOUBLET P1 3/2	A 96
C	IND=5 F1 DOUBLET SIGMA	A 97
C	IND F2 DOUBLET SIGMA	A 98
C		A 99
	READ (5,55) HV,LAM,NJ,GAM,IND	A 100
	READ (5,56) (DV(I),I=1,N)	A 101
	READ 56, (A(I),I=1,N)	A 102
C		A 103
C	READ ROTATIONAL LEVELS J	A 104
C		A 105
	READ (5,57) (J(I),I=1,NJ)	A 106
C		A 107
C	NEXT DATA CARD CONTAINS RE, THE INTERNUCLEAR EQUILIBRIUM DISTANCE.	A 108
C		A 109

C		A 111
	READ (5,58) D2	A 112
C		A 113
C	NEXT DATA CARD CONTAINS VSTART,VFIN,AND HDEF WHERE	A 114
C	TURNING POINTS ARE CALCULATED FROM VIBRATIONAL LEVEL. VSTART TO	A 115
C	VFIN IN STEPS OF HDEF F.G. FROM 0.5 TO 20.5 IN STEPS OF 1.0.	A 116
C		A 117
	READ (5,52) VSTART,VFIN,HDEF	A 118
C		A 119
C	NEXT CARD CONTAINS IOPEG.	A 120
C	SET IOPEG = 1, IF INTERMEDIATE STEPS IN THE EVALUATION OF THE	A 121
C	KLEIN ACTION INTEGRALS ARE TO BE PRINTED.	A 122
C	SET IOPEG = 0, IF INTERMEDIATE PRINT-OUT IS TO BE SKIPPED.	A 123
C	NORMALLY THE USER SHOULD SET IOPEG = 0.	A 124
C		A 125
	READ (5,50) IOPEG	A 126
	READ 60, D2	A 127
	READ 61, (D2(I),I=1,2)	A 128
C	THIS TERMINATES COMMENT CARDS ON THE PREPARATION OF DATA.	A 129
C	IF NO FURTHER PROBLEMS FOLLOW, REMEMBER TO ADD A BLANK CARD TO	A 130
C	THE DATA DECK.	A 131
C		A 132
C		A 133
	QIRA(2)=6HANGST.	A 134
	QIEN(2)=6H1/CM	A 135
	QIMS(1)=6HC12=12	A 136
	QIMS(2)=6H016=16	A 137
C		A 138
C	PRINT HEADING	A 139
C		A 140
	WRITE (6,51) (FMT(I),I=1,16)	A 141
	WRITE (6,51) (FMT(I),I=1,16)	A 141
C		A 142
C	PRINT THE MASSES AND THEIR UNITS.	A 143
C		A 144
	IF (ZMAS2) 10,10,0	A 145
9	WRITE (6,62) QIMS(IIMS),ZMAS1,ZMAS2	A 146
	GO TO 11	A 147
10	WRITE (6,63) QIMS(IIMS),ZMAS1	A 148
C		A 149
C		A 150
C	PRINT G(V) DATA, OR VIBRATIONAL CONSTANTS	A 151
C		A 152
11	IF (IQMK) 12,12,12	A 153
12	WRITE (6,DIERMT)	A 154
	WRITE (6,64) WF,WEXF,WEYF,WFZF,WETF	A 155
	GO TO 14	A 156
13	WRITE (6,65) QIEN(IEN)	A 157
	WRITE (6,66) (QI(I),I=1,N)	A 158
	WRITE (6,67)	A 159
C		A 160
C	PRINT RV DATA, OR ROTATIONAL CONSTANTS	A 161
C		A 162
14	IF (IQMK) 15,16,15	A 163
15	WRITE (6,DUEXT)	A 164

	WRITE (6,68) BE,ALPHA E,GAMMA E,DELTA E,EPSLNE	A 165
	GO TO 17	A 166
16	WRITE (6,69) QIEN(IEB)	A 167
	WRITE (6,70) (BVI(I),I=1,N)	A 168
	WRITE (6,67)	A 169
C		A 170
C	PRINT HEADING	A 171
17	WRITE (6,51) (FMT(I),I=1,16)	A 172
C		A 173
	IF (ZMAS2) 18,19,19	A 174
18	ZMU=ZMAS1	A 175
	GO TO 20	A 176
19	ZMU=ZMAS1*ZMAS2/(ZMAS1+ZMAS2)	A 177
20	ZIMS(1)=1.0	A 178
	ZIMS(2)=.0006704	A 179
	ZIRA(1)=1.0	A 180
	ZIRA(2)=1.889765	A 181
	ZMU=ZMU*ZIMS(1IMS)	A 182
	ZIEN(1)=ZMU*3.64366EF3	A 183
	ZIEN(2)=ZMU*1.6610926F-2	A 184
	ZIEN(3)=ZMU*1.339776F2	A 185
	FACH=60.201702/ZMU	A 186
	XI(1)=0.5	A 187
	DO 21 I=2,N	A 188
	IL=I-1	A 189
	YI(I)=XI(IL)+1.0	A 190
21	CONTINUE	A 191
	ZERO=0.0	A 192
C		A 193
C	CALCULATE THE BV TO BE USED IN LATER COMPUTATION OF POTENTIALS	A 194
C		A 195
	J1=0.	A 196
	DO 49 LJ=1,NJ	A 197
	J4=J(LJ)	A 198
	LAM2=LAM*LAM	A 199
C	IND=4 FOR TRIPLET SIGMA STATE	A 200
	GO TO (22,24,26,28,35,37,39,39), IND	A 201
C		A 202
C	SINGLET SIGMA ELECTRONIC STATES	A 203
C		A 204
22	J2=J4*(J4+1)	A 205
	DO 23 I=1,N	A 206
	BV(I)=BVI(I)-2.*BV(I)*J2+BV(I)*J2*J2	A 207
	BVF=BVI(I)*J2-BV(I)*J2*J2+BV(I)*J2*J2*J2	A 208
	G(I)=GI(I)+BVF	A 209
	GR(I)=G(I)	A 210
23	CONTINUE	A 211
	GO TO 41	A 212
C		A 213
C	DOUBLET PI 1/2 ELECTRONIC STATE - HILL AND VAN VLECK-	A 214
C		A 215
C	F1	A 216
24	JHAF2=(J4+.5)*J2.	A 217
	J3=2*J4+1	A 218
	J1=J4+(-1)**(IND+1)*.5	A 219

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DO 25 I=1,N
R=RV(I)SA1=A(I)SY1=A1/RSD=DV(I)
RV(I)=R*(1.-(4.*JHAF2+Y1*(Y1-4.)*LAM2)**-.5)-1/J3*(4.*D*J4**3.-.5*
1GAM)
RVE=R*(JHAF2-LAM2-.5*(4.*JHAF2+Y1*(Y1-4.)*LAM2)**.5)-D*J4**4.+.5*G
1AM*(J4+.5)
G(I)=G(I)+RVE
GR(I)=G(I)
25 CONTINUE
GO TO 41
C
C DOUBLET PI 3/2 ELECTRONIC STATE - HILL AND VAN VLECK-
C
C F2
26 JHAF2=(J4+.5)**2.
J1=J4+(-1)**(IND+1)*.5
J3=2*J4+1
DO 27 I=1,N
R=RV(I)SA1=A(I)SY1=A1/RSD=DV(I)
RV(I)=R*(1.+(4.*JHAF2+Y1*(Y1-4.)*LAM2)**-.5)-1./J3*(4*D*J4**3.+.5*
1GAM)
RVE=R*(JHAF2-LAM2+.5*(4.*JHAF2+Y1*(Y1-4.)*LAM2)**.5)-D*(J4+1.)*4.
1-.5*GAM*(J4+1.5)
G(I)=G(I)+RVE
GR(I)=G(I)
27 CONTINUE
GO TO 41
C
C TRIPLET SIGMA ELECTRONIC STATE
C
C A-IS COUPLING PARAMETER LAMDA,A IS EMPTY FOR THIS CALCULATION
C J(PROGRAM)=K(PHYSICAL)
C IFR=1 --- F1 ,IFR=2 --- F2 ,IFR=3 -- F3
28 IFR=2
GO TO (29,31,33), IFR
C
C F1
29 J3=2*J4+1
J2=J4*(J4+1)
DO 30 I=1,N
R=RV(I)SA1=A(I)SD=DV(I)
J4R=(2*J4+3)*R
TSQ=J4R*J4R-A1*A1-2*A1*R
TSQ=AMAX1(0.,TSQ)
TSQ=TSQ**-.5
RV(I)=R-2*D*J2+1/J3*(2*R-2*J4R*R/TSQ+GAM)
RVE=R*J2-D*J2*J2+J4R-A1-TSQ+GAM*(J4+1)
G(I)=G(I)+RVE
GR(I)=G(I)
30 CONTINUE
GO TO 41
C
C F2
31 J2=J4*(J4+1)
DO 32 I=1,N
R=RV(I)SA1=A(I)SD=DV(I)
RV(I)=R-2*D*J2

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	RVE=R*J2-D*J2*J2	A 275
	G(I)=G(I)+RVE	A 276
	GR(I)=G(I)	A 277
32	CONTINUE	A 278
	GO TO 41	A 279
C	F3	A 280
33	J2=J4*(J4+1)	A 281
	J3=2*J4+1	A 282
	DO 34 I=1,N	A 283
	R=BVI(I)*A1=A(I)*D=DV(I)	A 284
	J4R=(2*J4-1)*P	A 285
	TSQ=J4R*J4R+A1*A1-2*A1*P	A 286
	TSQ=AMAX1(0.,TSQ)	A 287
	TSQ=(TSQ)**.5	A 288
	RV(I)=R-2*D*J2+1/J3*(-2*P+2*J4R*R/TSQ-GAM)	A 289
	RVE=R*J2-J4R-A1+TSQ-GAM*J4-D*J2*J2	A 290
	G(I)=G(I)+RVE	A 291
	GB(I)=G(I)	A 292
34	CONTINUE	A 293
	GO TO 41	A 294
C		A 295
C	DOUBLET SIGMA ELECTRONIC STATE	A 296
C		A 297
C	A=GAM FOR THIS CALCULATION	A 298
C	J IS ACTUALLY K SINCE WE HAVE CASE B COUPLING	A 299
C	F1	A 300
35	J3=2*J4+1	A 301
	J2=J4*(J4+1)	A 302
	J1=J4	A 303
	DO 36 I=1,N	A 304
	R=BVI(I)*C=A(I)*D=DV(I)	A 305
	RV(I)=R*(1.-2.*D*J2/R-C/(2.*J3*R))	A 306
	RVE=R*J2-D*J2*J2-C*J2/2.	A 307
	G(I)=G(I)+RVE	A 308
	GR(I)=G(I)	A 309
36	CONTINUE	A 310
	GO TO 41	A 311
C	F2	A 312
37	J3=2*J4+1	A 313
	J2=J4*(J4+1)	A 314
	J1=J4	A 315
	DO 38 I=1,N	A 316
	R=BVI(I)*C=A(I)*D=DV(I)	A 317
	RV(I)=R*(1.-2.*D*J2/R+C/(2.*J3))	A 318
	RVE=R*J2+C*J4/2.-D*J2*J2	A 319
	G(I)=G(I)+RVE	A 320
	GR(I)=G(I)	A 321
38	CONTINUE	A 322
	GO TO 41	A 323
C		A 324
C	DOUBLET PI ELECTRONIC STATE - ALMY AND HORSEFALL -	A 325
C		A 326
C	OH X2PI IS INVERTED F2-(-)-J=K+1/2 AND F1-(+)-J=K-1/2	A 327
C	K IS READ IN MUST CONVERT TO J IND=7 FOR F2 IND=8 FOR F1	A 328
C	J(PROGRAM)=K(PHYSICAL) J1(PROGRAM)=J(PHYSICAL)	A 329

39	J1=J(LJ)+(-1)**(IND-1)*.5	A 330
	J2=J1*J1+J1	A 331
	DO 42 I=1,N	A 332
	R=RV(I)	A 333
	D=DV(I)	A 334
	C=A(I)	A 335
C	F=LAMDA=AV/RV	A 336
	F=C/R	A 337
C	F=MU=DV/RV	A 338
	F=D/R	A 339
	R1=R+2*D*J2-.5*D	A 340
C	RA=ALPHA**5	A 341
	R2=1+F*(4*J2+1-2*F)+F*F*(2*J2-.5)*(2*J2-.5)-F*F	A 342
	RA=(.25*F*F-F+1+(J2-.75)*R2)**.5	A 343
C	PARTIAL DERIVATIVE OF ALPHA = RP	A 344
	RP=.5/RA*(R2+(J2-.75)*(4*F+F*F*(4*J2-1)*2))	A 345
C	7=IND FOR F1 ,R=IND FOR F2	A 346
	RV(I)=R1+(-1)**IND*R*RP	A 347
	FE=R*(J2-.75)+D*(J2*J2-.5*J2+13/16)+R*RA*(-1)**IND	A 348
	G(I)=G(I)+FE	A 349
	GR(I)=G(I)	A 350
40	CONTINUE	A 351
C	PRINT K AND J THE ROTATIONAL QUANTUM NUMBERS FOR THIS PROBLEM	A 352
41	PRINT 71, J(LJ),J1	A 353
C		A 354
C	PRINT GV RV JUST CALCULATED	A 355
C		A 356
	WRITE (6,72) QIEN(IEN)	A 357
	WRITE (6,73) (G(I),I=1,N)	A 358
	WRITE (6,74) QIEN(IIEP)	A 359
	WRITE (6,75) (RV(I),I=1,N)	A 360
	PRINT 71, J(LJ),J1	A 361
C		A 362
C	FIND ZERO POINT VARIABLES	A 363
C		A 364
	NINT=1	A 365
	DO 42 I=1,6	A 366
	YX(I)=1	A 367
	YY(I)=DV(I)	A 368
	YYY(I)=G(I)	A 369
42	CONTINUE	A 370
	SIGH(I)=YX(I)	A 371
	NORDER=7	A 372
	MPTS=6	A 373
	CALL LSOPRT (XX,YY,NINT,NORDER,MPTS,SIGH,ANS)	A 374
	REQUIL=ANS(1)+ANS(2)*(0.5)+ANS(3)*(0.25)	A 375
	CALL LSOPRT (XX,YYY,NINT,NORDER,MPTS,SIGH,ANS)	A 376
	ZPTEN=ANS(1)+ANS(2)*(0.5)+ANS(3)*(0.25)	A 377
	RE=4.105853006/(REQUIL*ZMAS)**.5	A 378
	CALL RKT (RMIN,RMAX,MSTART,MFIN,NORD,MFIN,FV1,U,IOHK,IRHK,IOPEV,IO	A 379
	IDA,REQUIL,IOPEV)	A 380
C	ADD BLOCK OF PRINT OUT	A 381
C	REQUIRED ADDITIONAL DATA CARDS AT END OF DATA DECK	A 382
C	DISSOCIATION ENERGY - CARD 1 F9.2 D2	A 383
C	DISSOCIATION PRODUCTS - CARDS 2 A10 D3	A 384

	PRINT 51, (FMT(I),I=1,16)	A 385
	PRINT 76, (D3(I),I=1,2)	A 386
	D2F=D2/8066.02	A 387
	PRINT 77, 7MAS1,D2,D2F	A 388
	PRINT 78, J(LJ),J1	A 389
	PRINT 79	A 390
	PRINT 80	A 391
	ZE=0.0	A 392
	PRINT 81, ZE,ZF,RE,ZF,BEQUIL	A 393
	ASTAR=1H*	A 394
	PUNCH 51, (FMT(I),I=1,8)	A 395
	PUNCH 82	A 396
	L=0	A 397
	DO 44 I=1,NFIN	A 398
	G2=U(I)	A 399
	G1=G2/8066.02	A 400
	G3=G2/109737.039	A 401
	RMI=RMIN(I)	A 402
	RMA=RMAX(I)	A 403
	RM11=RMI/.529172	A 404
	RMA1=RMA/.529172	A 405
	VLEV=YI(I)	A 406
	CH=VLEV-INT(VLEV)	A 407
	IF (CH.GT..45.AND.CH.LT..55) GO TO 43	A 408
	PRINT 86, VLEV,G1,RMI,RMA,G2,ASTAR	A 409
	GO TO 44	A 410
43	L=L+1	A 411
	LI=L-1	A 412
	R1=RV(L)	A 413
	A1=A(L)	A 414
	D1=DV(L)	A 415
	R11=RV1(L)	A 416
	G21=G1(L)	A 417
	F=GR(L)	A 418
	F1=F/8066.02	A 419
	PRINT 85, VLEV,G1,RMI,RMA,G2,R1,F1,F,ASTAR,G21,R11,D1,A1,LI	A 420
	PUNCH 83, LI,G2	A 421
44	CONTINUE	A 422
	PUNCH 84, RE,ZF	A 423
	DO 45 I=1,NFIN	A 424
	PUNCH 84, RMIN(I),U(I),RMAX(I),U(I)	A 425
45	CONTINUE	A 426
	IF (LJ.GT.1) GO TO 46	A 427
	RM=RMIN(NFIN)-.2	A 428
	XMIN=AMAX1(0.,RM)	A 429
	XMAX=RMAX(NFIN)+1.	A 430
	YMAX=D2+20000.	A 431
	CALL MAPG (XMIN,XMAX,0.,YMAX,.1,1.,1.,1.)	A 432
	CALL ABSLINE (0.,0.,0.,1.)	A 433
	CALL ABSVECT (1.,1.)	A 434
	CALL ABSVECT (1.,0.)	A 435
	CALL ABSVECT (0.,0.)	A 436
	CALL ABSPEAK (.3,.05)	A 437
	CALL CHAROPT (0,0,0,0,0)	A 438
	CALL SYMBOL (10HRADIUS(ANGSTROMS)S.)	A 439

	CALL ABSPEAK (.25,.02)	A 440
	CALL SYMBOL (25HRKR POTENTIAL GENERATEDS.)	A 441
	CALL ABSPEAK (.65,.02)	A 442
	CALL SYMBOL (FMT)	A 443
	CALL ABSPEAK (.05,.4)	A 444
	CALL CHAROPT (0,0,0,1,0)	A 445
	CALL SYMBOL (14HENERGY(CM-1)S.)	A 446
46	V(1)=GR(1)	A 447
	V(1001)=RF	A 448
	V(2001)=RF	A 449
	DO 47 I=1,NFIN	A 450
	K=I+1	A 451
	V(K)=U(I)+GR(1)	A 452
	V(1000+K)=RMIN(I)	A 453
47	V(2000+K)=RMAX(I)	A 454
	NPTS=NFIN+1	A 455
	CALL LINES (V(1001),V(1),NPTS)	A 456
	CALL LINES (V(2001),V(1),NPTS)	A 457
	NL=J(LJ)	A 458
	CALL CHAROPT (0,0,0,0,0)	A 459
	CALL NUMBER (NL,7H2HJ=.13)	A 460
48	CONTINUE	A 461
	CALL FRAME	A 462
	GO TO 1	A 463
49	CALL EXIT	A 464
C		A 465
50	FORMAT (11)	A 466
51	FORMAT (8A10)	A 467
52	FORMAT (14,2F10,0)	A 468
53	FORMAT (214,4X,6A10)	A 469
54	FORMAT (5E10,0)	A 470
55	FORMAT (E10,4,11,13,F10,4,11)	A 471
56	FORMAT (8E10,0)	A 472
57	FORMAT (10I3)	A 473
58	FORMAT (F10,0)	A 474
59	FORMAT (3E10,0)	A 475
60	FORMAT (F9,2)	A 476
61	FORMAT (2A10)	A 477
62	FORMAT (77740H THE MASSES OF THE TWO ATOMS, BASED ON A6.6H, ARE F	A 478
	110.6,5H AND F10.6777)	A 479
63	FORMAT (77746H THE REDUCED MASS OF THE TWO ATOMS, BASED ON A6.5H,	A 480
	1 IS F10.6777)	A 481
64	FORMAT (63H0 THE G(V) CURVE IS CONSTRUCTED FROM THE FOLLOWING INPUT	A 482
	1T DATA. 777H WE = F10.3,8H, WEYE = F10.4,8H, WEYE = F10.3,8H, WEZE	A 483
	2=F10.3,8H, WEZE = F10.3)	A 484
65	FORMAT (32H THE INPUT G VALUES, ENERGY IN A6.18H, ARE GIVEN BELOW	A 485
	1,77)	A 486
66	FORMAT (1X10F11,3)	A 487
67	FORMAT (20X,48HVALUES OF -10, ARE TO BE FOUND BY INTERPOLATION.)	A 488
68	FORMAT (64H0 THE BV(V) CURVE IS CONSTRUCTED FROM THE FOLLOWING INPUT	A 489
	1T DATA. 777H BE = 1F11.5,10H, ALPHA = F11.4,10H, GAMMA = F11.4,	A 490
	210H, DELTA = F11.4,10H, EPSLNE = F11.4)	A 491
69	FORMAT (33H THE INPUT BV VALUES, ENERGY IN A6.18H, ARE GIVEN BELOW	A 492
	1W,77)	A 493
70	FORMAT (1X10F11,6)	A 494

71	FORMAT (4H1K= ,I3,4H J= ,F4.1)	A 495
72	FORMAT (61H THE FOLLOWING NUMBERS ARE THE MODIFIED G VALUES, ENER	A 496
	1GY IN ,A6,17H ARE GIVEN BELOW.//)	A 497
73	FORMAT (1X10F11.3)	A 498
74	FORMAT (46H THE FOLLOWING ARE THE MODIFIED RV, ENERGY IN A6,//)	A 499
75	FORMAT (1X10F11.6)	A 500
76	FORMAT (1H0,6X,29HDISSOCIATION PRODUCTS ARE ,2A10)	A 501
77	FORMAT (1H0,6X,13HREDUCED MASS=,F9.5,6X,21HDISSOCIATION ENERGY =,F	A 502
	10,2,6H 1/CM=,F9.4,3H EV)	A 503
78	FORMAT (1H0,5X,17HROTATIONAL LEVEL ,4X,2HK=,I5,7X,2HJ=,F5.1//)	A 504
79	FORMAT (28X,15HCALCULATED DATA,47X,17HEXPERIMENTAL DATA//)	A 505
80	FORMAT (4H V=,5X,6HGV(EV),3X,7HMIN(A),2X,7HMAX(A),3X,8HGV(1/CM)	A 506
	1,2X,8HBV(1/CM),3X,5HE(EV),3X,7HE(1/CM),4X,1H*,4X,8HGV(1/CM),3X,8HB	A 507
	2V(1/CM),3X,8HDV(1/CM),3X,8HAV(1/CM),3X,1HV//)	A 508
81	FORMAT (2X,F3.1,2X,F9.6,6X,F7.4,7X,F9.3,2X,F8.4)	A 509
82	FORMAT (11H KV,FTRIAL)	A 510
83	FORMAT (I10,F10.3)	A 511
84	FORMAT (4F12.5)	A 512
85	FORMAT (1H ,F4.1,2X,F9.6,2X,F7.4,2X,F7.4,2X,F9.3,2X,F8.4,2X,F6.3,3	A 513
	1X,F7.1,4X,A1,4X,F8.2,3X,F8.4,2X,F9.3,3X,F8.2,3X,I2)	A 514
86	FORMAT (1H ,F4.1,2X,F9.6,2X,F7.4,2X,F7.4,2X,F9.3,32Y,A1)	A 515
	END	A 516-

	SUBROUTINE PKR (RMIN,RMAX,VSTA,VFIN,HDEF,M,EV1,U,IQHK,IPHK,IOPEV,I	R	1
	IOPA,REOUIL,IOPEG)	R	2
C	PKR FINDS TURNING POINTS FROM G(V) AND RV DATA, OR FROM CONSTANT	R	3
	DIMENSION JEV(3000), EV(3000), RV(200), RI(3000), TEMP(200), U(200	R	4
	1), RMIN(200), RMAX(200), Y(200), Z(200), ZOC(9), MZ(5), IZ(5), IR(R	5
	240), IG(40)	R	6
	DIMENSION V(200), G(200), RI(200), DEV(200), OV(200), XG(20), YG(2	R	7
	0), ZG(20), EPSH(1), AGAUS(5,20), XGAUS(5,20), VSTA(1), VFIN(1), H	R	8
	2DED(1), FEND(20), FLF(1), ANS(3), YY(6), XFF(1), SIGH(1), XY(6), U	R	9
	3UU(200), T(40), HT(40), IX(30), UX(30)	R	10
	DIMENSION DEVP(200), OVP(200)	R	11
	COMMON Y,TEMP,JEV,EV,Q,NST,N,MST,D,XMIN,XMAX,INSC,MREG,NUSED,RI,NI	R	12
	1,NS,MAXIT,FACI,ZMU,DE,VF,WEXE,YEYF,WFEZ,WETF,BE,ALPHA, GAMMA,DELT	R	13
	2AE,VNIN,BQ,NG,GREP,UUU,RV,Z,ICK,H,K,HDEF,EPSLNF,XX,RRRRB,7PTFN,VL	R	14
	3V,LV,PF	R	15
	GFUNC(X)=(((((((WETF*X)+WFEZ)*X)+WEYF)*X)-WEXE)*X)+WF)*X	R	16
	BFUNC(X)=(((((((EPSLNF*X)+DELTA)*X)+GAMMA)*X)-ALPHA)*X)+BF	R	17
C	FAC = (HPLANCK*NAV/9*PI**2*C)**.5*E8/ZMU**.5	R	18
	FAC=4.1157859/SQRT(ZMU)	R	19
	NPROB=1	R	20
	MUST=P	R	21
	EV1=0.0	R	22
	CALL SECOND (BEGIN)	R	23
C		R	24
C	TURNING POINTS FOUND FOR V = VSTA,VFIN,HDEF.	R	25
C		R	26
C	INTERPOLATE G(V) AND RV DATA	R	27
C		R	28
	JJ=0	R	29
	JK=0	R	30
	IJ=0	R	31
	IK=0	R	32
	HDEF=.01	R	33
	MREG=1	R	34
	IF (IOPEV-1) 2,1,2	R	35
1	EV1=7(1)	R	36
2	WRITE (6,1-7) MUST	R	37
	DO 8 I=1,2	R	38
	IF (7(I)+10.) 3,0,2	R	39
3	IJ=IJ+1	R	40
	TEMP(IJ)=V(I)	R	41
	RI(IJ)=7(I)	R	42
	GO TO 5	R	43
4	JJ=JJ+1	R	44
	DEV(JJ)=V(I)	R	45
	IG(JJ)=1	R	46
5	IF (RV(I)+10.) 6,7,6	R	47
6	IK=IK+1	R	48
	RM(IK)=V(I)	R	49
	RMAX(IK)=RV(I)	R	50
	GO TO 3	R	51
7	JK=JK+1	R	52
	EV(JK)=V(I)	R	53
	IR(JK)=1	R	54
8	CONTINUE	R	55

	IF (JJ) 12,12,0	R	56
9	CALL NTRPSR (TEMP,U,UEV,PI,HDEF,IJ,JJ,VNIN,VN,INSC,MBEG,MUST)	R	57
	LOC=9	R	58
	IF (INSC) 07,10,07	R	59
10	DO 11 I=1,JJ	R	60
	IJ=IG(I)	R	61
	Z(IJ)=R1(I)	R	62
11	CONTINUE	R	63
12	IF (JK) 16,16,12	R	64
13	CALL NTRPSR (QMIN,RMAX,EV,PI,HDEF,IK,JK,VNIN,VN,INSC,MBEG,MUST)	R	65
	LOC=0	R	66
	IF (INSC) 07,14,07	R	67
14	DO 15 I=1,JK	R	68
	IK=IR(I)	R	69
	RV(IK)=R1(I)	R	70
15	CONTINUE	R	71
16	IF (IQHK) 17,10,17	R	72
17	EV1=-GEUNCF(0.5)	R	73
	IOPEV=0	R	74
	DO 18 I=1,N	R	75
	Z(I)=GEUNCF(Y(I))+EV1	R	76
18	CONTINUE	R	77
	GO TO 22	R	78
19	INTG=INTG	R	79
	MBEG=1	R	80
	M=1	R	81
	UEV(1)=0.	R	82
	HDEF=1.	R	83
	EV1=-EV1	R	84
	IF (EV1) 22,20,20	R	85
20	CALL NTRPSR (Y,Z,UEV,EV,HDEF,N,M,VNIN,VN,INSC,MBEG,MUST)	R	86
	LOC=1	R	87
	IF (INSC) 07,21,07	R	88
21	EV1=EV(1)	R	89
C	EV1 NOW CONTAINS THE ZERO POINT ENERGY BY EXTRAPOLATION.	R	90
	EV1=ZPTEN	R	91
22	IF (IRHK) 23,25,23	R	92
23	EV(1)=RF	R	93
	DO 24 I=1,M	R	94
	RV(I)=GEUNCF(Y(I))	R	95
24	CONTINUE	R	96
	GO TO 28	R	97
25	IF (IQRA) 26,27,26	R	98
26	EV(1)=REQUIL	R	99
	GO TO 28	R	100
27	CALL NTRPSR (Y,RV,UEV,EV,HDEF,N,M,VNIN,VN,INSC,MBEG,MUST)	R	101
C	EV(1) NOW CONTAINS RF BY EXTRAPOLATION	R	102
	LOC=7	R	103
	IF (INSC) 07,28,07	R	104
28	V(1)=0.	R	105
	G(1)=0.	R	106
	RO(1)=EV(1)	R	107
	DO 29 I=1,M	R	108
	V(I+1)=V(I)	R	109
	G(I+1)=G(I)	R	110

	PO(I+1)=PV(I)	D	111
29	CONTINUE	D	112
	NP=NP+1	D	113
	IF (IOPRV) 30,31,30	D	114
30	CONTINUE	D	115
	EV1=EV1+G(2)	D	116
31	DO 32 I=2,NP	D	117
	G(I)=G(I)-EV1	D	118
	V(I)=V(I)	P	119
	Z(I)=G(I)	D	120
	PV(I)=PO(I)	D	121
32	CONTINUE	D	122
	IF (IOPRV) 33,34,33	D	123
33	EV1=-G(2)	D	124
34	IF (NPOR-17) 37,35,37	D	125
35	M=1	D	126
	EV(I)=OF	D	127
	CALL MTRPS (Z,V,EV,HEV,HOF,NP,M,VNIN,VN,INSC,MREG,MUST)	D	128
	LCC=2	D	129
	IF (INSC) 37,36,37	D	130
36	NP=NP+1	D	131
	V(NP)=HEV	D	132
	V(NP)=HEV	D	133
	Z(NP)=OF	D	134
	G(NP)=OF	D	135
	PO(NP)=0.	P	136
	PV(NP)=0.	D	137
37	V(I)=0.	D	138
	Z(I)=0.	D	139
	PV(I)=PO(I)	D	140
	VNIN=VSTA	D	141
	VN=VFIN	D	142
	HOF=HOFD	D	143
	M=0	D	144
	WRITE (6,102) (V(I),Z(I),I=1,NP)	D	145
	WRITE (6,100) (V(I),PV(I),I=1,NP)	D	146
	IF (IOPV) 30,40,30	D	147
38	M=(VFIN-VSTA)/HOFD+1.	D	148
	DO 39 I=1,M	D	149
	OFV(I)=VSTA+FLOAT(I-1)*HOFD	D	150
	OFVSR=OFV(I)	D	151
	OV(I)=OFUNCF(OFVSR)	D	152
	OPR(I)=OV(I)	D	153
	OFVR(I)=OFV(I)	D	154
39	CONTINUE	D	155
	INSC=0	D	156
	GO TO 41	D	157
40	CALL MTRPS (V,G,OFV,OV,HOFD,NP,M,VSTA,VFIN,INSC,MREG,MUST)	D	158
	LCC=2	D	159
	WRITE (6,110) HOF,VMIN,VN,MREG,MUST,INSC,NP,M	D	160
41	WRITE (6,111)	D	161
	PRINT 112, (OFV(I),OV(I),I=1,M)	D	162
	IF (INSC) 37,42,37	D	163
42	DO 43 I=1,M	D	164
	OFV(I)=OFV(I)	D	165

43	U(1)=OV(1)	R	166
C	CONTINUE	R	167
C		R	168
C	INTEGRATION CONSTANTS	R	169
		R	170
	STEP=.0	R	171
	VZ(1)=101	R	172
	VZ(2)=81	R	173
	VZ(3)=61	R	174
	IZ(1)=8	R	175
	XGAUS(1,1)=.019855071751232	R	176
	XGAUS(1,2)=.101646761293186	R	177
	XGAUS(1,3)=.237233795041826	R	178
	XGAUS(1,4)=.408282679752175	R	179
	XGAUS(1,5)=1.-XGAUS(1,4)	R	180
	XGAUS(1,6)=1.-XGAUS(1,3)	R	181
	XGAUS(1,7)=1.-XGAUS(1,2)	R	182
	YGAUS(1,8)=1.-XGAUS(1,1)	R	183
	AGAUS(1,1)=.050614269145188	R	184
	AGAUS(1,2)=.111190517226697	R	185
	AGAUS(1,3)=.156853322939044	R	186
	AGAUS(1,4)=.181241891609181	R	187
	AGAUS(1,5)=AGAUS(1,4)	R	188
	AGAUS(1,6)=AGAUS(1,3)	R	189
	AGAUS(1,7)=AGAUS(1,2)	R	190
	AGAUS(1,8)=AGAUS(1,1)	R	191
	IZ(2)=6	R	192
	XGAUS(2,1)=.033765242998424	R	193
	XGAUS(2,2)=.160395306766868	R	194
	XGAUS(2,3)=.380690406058402	R	195
	XGAUS(2,4)=1.-XGAUS(2,3)	R	196
	XGAUS(2,5)=1.-XGAUS(2,2)	R	197
	XGAUS(2,6)=1.-XGAUS(2,1)	R	198
	AGAUS(2,1)=.085662246189585	R	199
	AGAUS(2,2)=.180380786524070	R	200
	AGAUS(2,3)=.233056067206345	R	201
	AGAUS(2,4)=AGAUS(2,3)	R	202
	AGAUS(2,5)=AGAUS(2,2)	R	203
	AGAUS(2,6)=AGAUS(2,1)	R	204
	IZ(3)=4	R	205
	XGAUS(3,1)=.060431846202974	R	206
	YGAUS(3,2)=.330000479207572	R	207
	YGAUS(3,3)=1.-YGAUS(3,2)	R	208
	YGAUS(3,4)=1.-YGAUS(3,1)	R	209
	AGAUS(3,1)=.173027422569727	R	210
	AGAUS(3,2)=.326072577431273	R	211
	AGAUS(3,3)=AGAUS(3,2)	R	212
	AGAUS(3,4)=AGAUS(3,1)	R	213
	ZG(1)=ZG(3)	R	214
	WRITE (6,113)	R	215
	DO 94 I=1,M	R	216
	TEMP1=OV(I)	R	217
	MUS2=MUS1/2	R	218
	NR=MUS2+1	R	219
	NF=N-NR+1	R	220

	DO 44 J=NR,NF	R 221
	IF (TEMP1-V(J)) 45,45,44	R 222
44	CONTINUE	R 223
	ISG=NF+1	R 224
	GO TO 46	R 225
45	ISG=J	R 226
46	NSTA=ISG-NUS2	R 227
	VMIN=0.	R 228
	EEG=1.	R 229
	GEG=0.	R 230
	LT=1	R 231
	I7GD=0	R 232
	GDO=0.	R 233
	FDO=0.	R 234
	ISG=0	R 235
	ISR=0	R 236
C		R 237
C	COMMENCE FINDING TURNING POINTS BY INTEGRATION	R 238
C		R 239
	CALL SECOND (BEG1A)	R 240
47	RS=VMIN+(TEMP1-VMIN)*STEP	R 241
	IF (LT=3) 48,48,57	R 242
48	MQ=M2(LT)	R 243
	KM=(MQ-1)/2	R 244
	TMIN=VMIN	R 245
	TS=RS	R 246
	A=(TS-TMIN)/ELDATE(MQ-1)	R 247
	MX=0	R 248
	IF (IQHK) 100,49,100	R 249
49	CALL NTPSP (Y,Z,HEV,FV,A,ND,MY,TMIN,TS,INSC,MPEG,MUST)	R 250
	LOC=3	R 251
	IF (INSC) 97,50,97	R 252
50	IF (GDO) 53,51,53	R 253
51	MX=0	R 254
	IF (IRUK) 102,52,102	R 255
52	CALL NTPSP (Y,RV,HEV,PI,A,ND,MY,TMIN,TS,INSC,MPEG,MUST)	R 256
	LOC=4	R 257
	IF (INSC) 97,53,97	R 258
53	DO 55 J=1,MQ	R 259
	DFNO=U(1)-EV(J)	R 260
	IF (DFNO) 99,99,54	R 261
54	HEV(J)=1./SQRT(DFNO)	R 262
	FV(J)=PI(J)*HEV(J)	R 263
55	CONTINUE	R 264
	ESUM=HEV(1)+4.*HEV(2)+HEV(MQ)	R 265
	GSUM=FV(1)+4.*FV(2)+FV(MQ)	R 266
	DO 56 J=2,KM	R 267
	ESUM=ESUM+4.*HEV(2*J)+2.*HEV(2*J-1)	R 268
	GSUM=GSUM+4.*FV(2*J)+2.*FV(2*J-1)	R 269
56	CONTINUE	R 270
	EF(2)=A*ESUM/3.	R 271
	GF(2)=A*GSUM/3.	R 272
	IF (LT=1) 56,56,79	R 273
57	I7DC=(LT-1)/2	R 274
	IF (I7DC=3) 59,59,59	R 275

58	I2DO=3	R 276
59	NGAS=17(I2DO)	R 277
	DO 60 J=1,NGAS	R 278
	XG(J)=(RS-VMIN)*XGAUS(I2DO,J)+VMIN	R 279
	UEV(J)=XG(J)	R 280
60	CONTINUE	R 281
	MST=1	R 282
	EPSH=TEMP1-XG(NGAS)	R 283
	FEPS=EPSH	R 284
	IF (EPSH(1)) 93,61,62	R 285
61	IF (EPSH(2)) 93,93,62	R 286
62	IF (IQHK) 104,63,104	R 287
63	CALL NTRPSR (V,G,XG,YG,EP SH,ND,NGAS,VMIN,RS,INSC,MST,NUST)	R 288
	LOC=5	R 289
	IF (INSC) 97,64,97	R 290
64	IF (I2GD) 65,65,75	R 291
65	IF (GDO) 68,66,68	R 292
66	MST=1	R 293
	IF (IRHK) 105,67,105	R 294
67	CALL NTRPSR (Y,BV,UEV,BI,FEPS,ND,NGAS,TMIN,TS,INSC,MST,NUST)	R 295
	LOC=6	R 296
	IF (INSC) 97,69,97	R 297
68	FSUM=0.0	R 298
	GSUM=0.0	R 299
	DO 72 J=1,NGAS	R 300
	IF (IQHK) 70,69,70	R 301
69	DENO(J)=OV(I)-YG(J)	R 302
70	IF (DENO(J)) 99,99,71	R 303
71	XG(J)=AGAUS(I2DO,J)/SQRT(DENO(J))	R 304
	YG(J)=BI(J)*XG(J)	R 305
	FSUM=FSUM+XG(J)	R 306
	GSUM=GSUM+YG(J)	R 307
72	CONTINUE	R 308
	IF (BI(NGAS)-BI(1)) 74,73,74	R 309
73	I2GD=1	R 310
74	RSV=RS-VMIN	R 311
	FEG2=RSV*FSUM	R 312
	GEG2=RSV*GSUM	R 313
	GO TO 78	R 314
75	FSUM=0.0	R 315
	DO 77 J=1,NGAS	R 316
	DENO=OV(I)-YG(J)	R 317
	IF (DENO) 99,99,76	R 318
76	XG(J)=AGAUS(I2DO,J)/SQRT(DENO)	R 319
	FSUM=FSUM+XG(J)	R 320
77	CONTINUE	R 321
	GSUM=BI(NGAS)*FSUM	R 322
	GO TO 74	R 323
78	IF (FEG2/FEG-1,F-6) 79,79,80	R 324
79	FDO=1.	R 325
80	IF (GEG2/GEG-1,F-6) 81,81,82	R 326
81	GDO=1.	R 327
82	IF (ABSF(FEG2/FEG1)-.9) 84,84,83	R 328
83	FDO=1.	R 329
84	IF (ABSF(GEG2/GEG1)-.9) 86,86,85	R 330

85	GDO=1.	R	231
86	LT=LT+1	R	232
	FEG1=FEG2	R	233
	GEG1=GEG2	R	234
	IF (FDO) 88,87,88	R	235
87	FEG=FEG+FEG2	R	236
	IF (GDO) 90,89,90	R	237
88	IF (GDO) 93,89,93	R	238
89	GEG=GEG+GEG2	R	239
90	VMIN=BS	R	240
	IF (IOPEG) 91,92,91	R	241
91	CALL SECOND (AFTEA)	R	242
	XTIQ=(AFTEA-REGIA)	R	243
	REGIA=AFTEA	R	244
	WRITE (6,114) FEG,GEG,XTIQ	R	245
92	IF (LT-20) 47,47,98	R	246
93	F=FEG*FAC	R	247
	GF=GEG/FAC	R	248
	RMAX(I)=SQRT(F*F+F/GF)+F	R	249
	RMIN(I)=RMAX(I)-2.*F	R	250
	CALL SECOND (AFTER)	R	251
	XTIQ=AFTER-REGIN	R	252
	REGIN=AFTER	R	253
C	WRITEOUTPUTTAP6,104,TEMP1,U(I),RMIN(I),RMAX(I),XTIQ,PI(NGAS)	R	254
	TEMP1I=TEMP1	R	255
	WRITE (6,115) TEMP1I,U(I),RMIN(I),RMAX(I),XTIQ,PI(NGAS),F,GF	R	256
94	CONTINUE	R	257
	DO 95 I=1,N	R	258
	Z(I)=Z(I+1)	R	259
	Y(I)=Y(I+1)	R	260
	PV(I)=PV(I+1)	R	261
95	CONTINUE	R	262
	WRITE (6,113)	R	263
96	RETURN	R	264
97	ZOC(1)=6H FV1	R	265
	ZOC(2)=6H G(LFV)	R	266
	ZOC(3)=6H S.P.FV	R	267
	ZOC(4)=6H S.P.PV	R	268
	ZOC(5)=6H D.P.FV	R	269
	ZOC(6)=6H D.P.PV	R	270
	ZOC(7)=6H RV1	R	271
	ZOC(8)=6H S FILL	R	272
	ZOC(9)=6H RV FILL	R	273
	WRITE (6,116) ZOC(LOC),U(I)	R	274
	INTG=1	R	275
	GO TO 94	R	276
98	WRITE (6,117)	R	277
	INTG=1	R	278
	GO TO 96	R	279
99	INTG=1	R	280
	WRITE (6,118)	R	281
	GO TO 96	R	282
100	MX="0	R	283
	DO 101 J=1,M0	R	284
	DEV(J)=MIN(N+FLCATE(J-1))*A	R	285

	EV(J)=GEUNCF(UFV(J))	R 386
101	CONTINUE	R 387
	GO TO 50	R 388
102	MX=MQ	R 389
	DO 103 J=1,MQ	R 390
	UEV(J)=TMIN+FLOAT(J-1)*A	R 391
	RI(J)=REUNCF(UEV(J))	R 392
103	CONTINUE	B 393
	GO TO 53	R 394
104	CALL DGUNC (XG,DENQ,NGAS,TEMP1)	R 395
	GO TO 64	R 396
105	DO 106 J=1,NGAS	R 397
	RI(J)=REUNCF(UEV(J))	R 398
106	CONTINUE	R 399
	GO TO 68	B 400
C		R 401
107	FORMAT (20H0 NUSED IN RESRKR = 12,1H.)	R 402
108	FORMAT (32H0 THE G(V) VALUES USED BELOW ARE//,6X,6(2X,1HV7X,1HG10X	R 403
	1),/,6(F10.1,F11.4)))	R 404
109	FORMAT (33H0 THE BV(V) VALUES USED BELOW ARE//,6X,6(2X,1HV6X,2HBV1	R 405
	10X),/,6(F10.1,F11.7)))	B 406
110	FORMAT (6H0HDFS=1PF15.7,7H, VMIN=E15.7,5H, VN=E15.7,7H, MREG=15/9X	B 407
	1,7H, MUST=15,7H, INSC=15,4H, N=15,4H, M=15)	R 408
111	FORMAT (54H0 OUTPUT V,G--LEVELS AT WHICH TURNING POINTS ARE FOUND/	B 409
	1/,6X,6(2X,1HV7X,1HG10X)/)	R 410
112	FORMAT (6(F10.1,F11.4))	R 411
113	FORMAT (1H1)	R 412
114	FORMAT (6X,6HFEF = 1PF15.7,8H, GEG = E15.7,10X,SHREQUIRED OPER,3,9	R 413
	1H SECONDS.)	R 414
115	FORMAT (10H0 FOR V = F5.1,3X,6H G = F10.2,14H 1/CM, RMIN = F10.7,	R 415
	112H AND RMAX = F10.7,27H ANGSTROMS. THIS REQUIRED F8.3,9H SECONDS	R 416
	2,7/20X,12H ALSO, BV = F12.7/20X,49H THE KLEIN ACTION INTEGRALS F AN	R 417
	3D G ARE EQUAL TO 2F15.9/77)	R 418
116	FORMAT (26H0 NTRPDP UNSUCCESSFUL FOR A6,11H, WHEN U = F16.8)	B 419
117	FORMAT (20H0 TEG REACHED MAXIT)	R 420
118	FORMAT (22H0 DENQ IS NOT POSITIVE)	R 421
	END	R 422-

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SUBROUTINE NTRPSR (XJ,YJ,YO,YO,XN,N,K,XMIN,XMAX,INSC,MPEG,NUSED) C 1
NTRPSR INTERPOLATION PROGRAM (BY SUCCESSIVE RANGES) SINGLE PREC. C 2
C C 3
C THE METHOD OF LAGRANGE IS USED. THE INPUT POINTS NEED NOT BE C 4
C EQUALLY SPACED. THERE ARE TWO MODES OF INPUT AVAILABLE. THE C 5
C FIRST OCCURS WHEN M = 0. THE ABSCISSAE ARE THEN GENERATED FROM C 6
C XMIN,XMAX,AND XH. AT EXIT M = NO. OF POINTS FOUND, AND XO C 7
C CONTAINS THE ABSCISSAE. M WILL BE CHECKED TO INSURE THAT THE C 8
C DIMENSION IS NOT EXCEEDED. MDIMM = THE DIMENSION OF THE XO, YO C 9
C ARRAYS. THE SECOND MODE OCCURS WHEN M IS POSITIVE. THE M C 10
C ABSCISSAE ARE THEN ASSUMED TO HAVE BEEN GENERATED PRIOR TO C 11
C ENTRY. THE STARTING INDEX FOR THE OUTPUT ARRAY MUST BE C 12
C SPECIFIED. THE FIRST POINT FOUND WILL BE AT XO(MPEG). XH MUST C 13
C BE GIVEN SINCE THE ORDINATE FOR ANY POINT CLOSER THAN .01*XH TO C 14
C AN INPUT POINT IS TAKEN AS THAT FOR THE INPUT POINT. -NUSED- IS C 15
C THE NUMBER OF POINTS USED FOR EACH INTERPOLATED POINT. *NUSED* C 16
C MUST BE EVEN AND LESS THAN OR EQUAL TO -N-. NUSED = 8 IS C 17
C SUGGESTED. ANY POINT FARTHER THAN NUSED/2 POINTS FROM EITHER END C 18
C IS FOUND FROM THE NUSED/2 ON EACH SIDE. NTRPSR WILL SCALE AND C 19
C RESCALE IN ORDER TO AVOID OVERFLOW. IF THE FIRST SCALING DOES C 20
C NOT SUCCEED, NTRPSR WILL TRY UP TO 7 TIMES MORE BEFORE RETURNING C 21
C IN THE ERROR MODE. (INSC = 1) C 22
C INPUT IS XJ,YJ,(XO),XH,N,M,(XMIN),(XMAX),MPEG,NUSED. C 23
C OUTPUT IS (XO),YO,INSC. C 24
C INSC = 0 IF PROGRAM WAS SUCCESSFUL. IF NOT, INSC = 1. C 25
C C 26
C DIMENSION XI(200), YI(200), XO(3000), YO(3000), XJ(200), YJ(200), C 27
C INUMB(200) C 28
C MDIMM=3000 C 29
C XMAX=XMAX C 30
C XMIN=XMIN C 31
C XH=ARISE(XH) C 32
C M=X C 33
C IREV=0 C 34
C IPFX=0 C 35
C M IS ZERO. IF XH, XMIN, XMAX ARE TO BE USED. IF M IS NOT = TO C 36
C ZERO, THEN XO(I), I = 1,M WILL BE USED AS ABSCISSA. C 37
C IF (M) 32,1,6 C 38
C M=XINTF(ARISE((XMAX-XMIN)/XH))+1 C 39
C IF M IS MORE THAN DIMENSION OF XO, RETURN IN ERROR MODE. C 40
C IF (M+MPEG-MDIMM-2) 2,33,33 C 41
C M=MPEG+M-1 C 42
C IF (XMAX-XMIN) 2,4,4 C 43
C XMIN=XMAX C 44
C XMAX=XMIN C 45
C IREV=1 C 46
C DO 5 I=MPEG,M C 47
C XO(I)=FLOAT(I-MPEG)*XH+XMIN C 48
C CONTINUE C 49
C DO 7 I=1,M C 50
C XI(I)=XJ(I) C 51
C CONTINUE C 52
C M=MPEG+M-1 C 53
C MSTA=MPEG C 54
C MUST=NUSED/2 C 55

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	NS=NUST+1	C 56
	NF=N-NS+1	C 57
	NFP=NFP+1	C 58
	DO 9 I=NS,NFP	C 59
	NUMB(I)=0	C 60
R	CONTINUE	C 61
	IF (XO(MF)-XO(MREG)) 9,11,11	C 62
9	M2=M/2	C 63
	M2F=MREG+M2-1	C 64
	DO 10 I=MREG,M2F	C 65
	K=MF+MREG-I	C 66
	TEMP=XO(I)	C 67
	XO(I)=XO(K)	C 68
	XO(K)=TEMP	C 69
10	CONTINUE	C 70
	IREV=1	C 71
11	IF (XI(N)-XI(1)) 12,14,14	C 72
12	N2=N/2	C 73
	DO 13 I=1,N2	C 74
	K=N+1-I	C 75
	TEMP=XJ(I)	C 76
	TEMS=YJ(I)	C 77
	XJ(I)=XJ(K)	C 78
	YJ(I)=YJ(K)	C 79
	XJ(K)=TEMP	C 80
	YJ(K)=TEMS	C 81
13	CONTINUE	C 82
	IREX=1	C 83
14	IF (NF-NS) 19,19,15	C 84
15	DO 16 J=MREG,MF	C 85
	DO 17 I=NS,NF	C 86
	IF (XO(J)-XI(I)) 16,16,17	C 87
16	NUMB(I)=NUMB(I)+1	C 88
	GO TO 18	C 89
17	CONTINUE	C 90
	NUMB(NFP)=NUMB(NFP)+1	C 91
18	CONTINUE	C 92
	GO TO 20	C 93
19	NUMB(NFP)=0	C 94
20	M=C	C 95
	DO 24 L=NS,NFP	C 96
	IF (NUMB(L)) 24,24,21	C 97
21	M=NUMB(L)	C 98
	NSTA=L-NUST	C 99
	GO TO 35	C 100
22	IF (INSC) 24,22,24	C 101
23	NSTA=NSTA+M	C 102
24	CONTINUE	C 103
25	K=NSTA-MREG	C 104
	IF (IREV) 28,22,26	C 105
26	M2F=K/2+MREG-1	C 106
	DO 27 I=MREG,M2F	C 107
	J=MF+MREG-I	C 108
	TEMP=XO(I)	C 109
	TEMS=YO(I)	C 110

	XO(I)=XO(J)	C 111
	YO(I)=YO(J)	C 112
	YO(J)=TEMP	C 113
	YO(J)=TEMS	C 114
27	CONTINUE	C 115
28	IF (IREX) 21,21,29	C 116
29	DO 30 I=1,N2	C 117
	J=N-1-2	C 118
	J=N+1-1	C 119
	TEMP=XJ(I)	C 119
	TEMS=YJ(I)	C 120
	XJ(I)=XJ(J)	C 121
	YJ(I)=YJ(J)	C 122
	XJ(J)=TEMP	C 123
	YJ(J)=TEMS	C 124
30	CONTINUE	C 125
31	RETURN	C 126
32	WRITE (6,51)	C 127
	INSC=1	C 128
	GO TO 25	C 129
33	H=(XMAX-XMIN)/FLOATE(NOINM-MREG)	C 130
	WRITE (6,52) H	C 131
	INSC=1	C 132
	GO TO 25	C 133
34	WRITE (6,53) L	C 134
	GO TO 25	C 135
35	NCON=1	C 136
	DEFA=1.414214	C 137
	NFIN=NSTA+NUSED-1	C 138
	DO 36 I=NSTA,NFIN	C 139
	XI(I)=XJ(I)	C 140
	YI(I)=YJ(I)	C 141
36	CONTINUE	C 142
	NSTA=NSTA+1	C 143
	XSCALE=(XI(NFIN)-XI(NSTA))/10.	C 144
	YMAX=YI(NSTA)	C 145
	YMIN=YI(NSTA)	C 146
	DO 37 I=NSTA,NFIN	C 147
	YMAX=MAX1F(YMAX,YI(I))	C 148
	YMIN=MIN1F(YMIN,YI(I))	C 149
37	CONTINUE	C 150
	YSCALE=YMAX-YMIN	C 151
	DO 38 I=NSTA,NFIN	C 152
	XI(I)=XI(I)/XSCALE	C 153
	YI(I)=(YI(I)-YMIN)/YSCALE+.5	C 154
38	CONTINUE	C 155
	XH=ARSE(XN)/XSCALE	C 156
	NFIN=NSTA+N-1	C 157
	NSTA=NSTA	C 158
39	EDSIL=.77458	C 159
	DO 44 I=NSTA,NFIN	C 160
	YO(I)=XO(I)/XSCALE	C 161
	YO(I)=0.0	C 162
	EDUM=1.0	C 163
	DO 44 I=NSTA,NFIN	C 164

C	FIND XO(II)-XI(I) FOR NUMERATOR AND CHECK FOR NEARNESS.	C 165
	XNUM=XO(II)-XI(I)	C 166
	IF (ABS(XNUM)-EPSIL) 40,40,41	C 167
40	YO(II)=YI(I)	C 168
	GO TO 45	C 169
C	PNUM = PRODUCT OF ALL XNUM	C 170
41	PNUM=PNUM*XNUM	C 171
C	CONSTRUCT DENOMINATOR AND SUM	C 172
	DDEN=1.0	C 173
	DO 42 J=NSTA,NFIN	C 174
	IF (I-J) 42,42,42	C 175
42	DDEN=(XI(I)-XI(J))*DDEN	C 176
	IF QUOTIENT OVERFLOW 47,43	C 177
43	CONTINUE	C 178
	DEN=DDEN*XNUM	C 179
	YO(II)=YI(I)/DEN+YO(II)	C 180
	IF ACCUMULATOR OVERFLOW 50,44	C 181
44	CONTINUE	C 182
	YO(II)=YO(II)*PNUM	C 183
45	YO(II)=(YO(II)-.5)*YSCALE+YMIN	C 184
	XO(II)=YO(II)*XSCALE	C 185
46	CONTINUE	C 186
	INSC=0	C 187
	GO TO 22	C 188
47	WRITE (6,54) NCON,XSCALE	C 189
	WRITE (6,55) II,I,J	C 190
	NCON=NCON+1	C 191
	DO 48 I=NSTA,NFIN	C 192
	XI(I)=XI(I)/REFA	C 193
48	CONTINUE	C 194
	XO(II)=XO(II)*XSCALE	C 195
	MTA=II	C 196
	XH=XH/REFA	C 197
	XSCALE=XSCALE*REFA	C 198
	IF (NCON-P) 39,39,40	C 199
49	INSC=1	C 200
	GO TO 22	C 201
50	WRITE (6,56)	C 202
	INSC=1	C 203
	GO TO 22	C 204
C		C 205
51	FORMAT (44H0 ERROR IN INPUT TO NTRPS. M IS NEGATIVE.)	C 206
52	FORMAT (58H0 ERROR IN INPUT TO NTRPS. MINIMUM ALLOWABLE SPACING	C 207
	IS 12.7)	C 208
53	FORMAT (43H0 INTR1 WAS UNABLE TO INTERPOLATE IN RANGE I2)	C 209
54	FORMAT (8H NCON =I3,I1H, XSCALE = F10.7)	C 210
55	FORMAT (26H OVERFLOW OCCURRED AT II=I4,4H I=I2,4H J=I2)	C 211
56	FORMAT (48H0 ACCUMULATOR OVERFLOW. DEN MUST BE TOO SMALL.)	C 212
	END	C 213-

	SUBROUTINE DGUNC (XG,DENO,NGAS,TEMP1)	D	1
C	DGUNC FINDS G(V) = G(V-X)	D	2
	DIMENSION XG(20), DENO(20)	D	3
	DIMENSION UEV(1000), EV(3000), BV(200), RI(3000), TEMP(200), U(200	D	4
	1), Y(200), Z(200)	D	5
	COMMON Y,TEMP,UEV,EV,D,NST,N,MST,M,XMIN,XMAX,INSC,MBEG,NUST,RI,NI,	D	6
	INS,MAXIT,FACH,7*U,DE,WE,WEXE,WEYE,WEZE,WETE,BE,ALPHA, GAMMA,DELTA	D	7
	2F,VNIN,BQ,WQ,SPED,U,PV,Z,ICK,H,K,HDFS,FPSLNE	D	8
	V=TEMP1	D	9
	VA=V*V	D	10
	VB=VA*V	D	11
	VC=VB*V	D	12
	DO 1 I=1,NGAS	D	13
	Y=TEMP1-XG(I)	D	14
	X=Y	D	15
	XA=X*X	D	16
	XB=XA*X	D	17
	XC=XB*X	D	18
	DENO(I)=WE*X+(XA-2.*V*X)*WEXE+((VA*X-V*XA)*3.+XB)*WEYE+((VB*X+V*XB	D	19
	1)*4.-6.*VA*XA-XC)*WEZE+((VC*X-V*XC)*5.+(VA*XB-VB*XA)*10.)*WETE	D	20
1	CONTINUE	D	21
	RETURN	D	22
	END	D	23-

APPENDIX II

COMPUTER PROGRAM FRANKON

The program FRANKON was used at AFWL to calculate Franck-Condon factors, r centroids, r^2 centroids. A listing of this program is included in this appendix along with an explanation of the input data and a sample data deck.

1. INPUT DATA

The reduced mass of the molecule or the mass of each atom is needed. These can be based on either C_{12} or O_{16} . A good source for reduced masses based on O_{16} is Herzberg (Ref. 31). The vibrational potential of the lower electronic state and the vibrational potential of the upper electronic state is read into the program. The value of the internuclear separation r and the potential $v(r)$ may be read in any one of several different units. The potential to be read in can be obtained from the output of program TURNPT or it can be taken from potentials which have been published. There is also the option of generating an analytic potential by programming the desired expressions and putting these in subroutine POTGEN.

Also needed are the dissociation energies of the upper and lower electronic states and the energies of the various vibrational levels for which one wishes to calculate Franck-Condon factors. The Franck-Condon factors can be calculated for any desired rotational level by specifying appropriate values for JROTL, JROTU. The energies of the rotationless vibrational levels are then adjusted by adding the appropriate rotational energy given by

$$E_R = \left\{ B_e + \alpha_e (v+1/2) + \gamma_e (v+1/2)^2 \right\} \frac{J(J+1)}{\left(\frac{h N_o \mu}{8\pi^2 c a_o^2} \right)}$$

where the constants B_e , α_e , γ_e are read in for the lower and upper states. The separation of the minimums of the two states, T_e , is also read in.

2. DATA DECK

As in the case of program TURNGPT, Zare has made extensive use of comment cards in program FRANKON and little or no explanation is needed to explain how to set up the data deck.

Card Number

1	ITEST I1	1 in column one if problem is to follow
2	Title 72H1	carriage control in column 1, name of problem in columns 1-72
3	IIMS, ZMAS1, ZMAS2, I4, 2F10.0	IIMS = 1 mass based on C = 12 IIMS = 2 mass based on O = 16 ZMAS1 mass of first atom (reduced mass of molecule) ZMAS2 mass of second atom (or zero when using reduced mass)
(for lower state)		
4	IIRA, IIEN, N(IKON) 3I4	IIRA = units used for internuclear separation IIRA = 1 atomic units (a_0) IIRA = 2 Angstrom units (\AA) IIEN = units used for energy IIEN = 1 atomic units (hartree) IIEN = 2 1/cm (kayser) IIEN = 3 electron volt N(IKON) = number of data points for potential to be read in
5 through 5+N(1)	XI, YI Format in columns 13-72 of Card 4	XI - internuclear separation in units at IIRA YI - energy of corresponding point of potential in units of IIEN

Card Number

6+N(1)	NDE, DE(IKON) I4, F10.0	NDE = 0 if zero point of the potential is at $R = \infty$ NDE = 1 if zero point of the potential is at $R = R_e$
7+N(1)	XMIN, XMAX, XH, IIRA 3F100, I4	XMIN, XMAX the minimum and maxi- mum value of internuclear separa- tion at which the wave functions were calculated, with mesh spacing of XH all in units of IIRA
8+N(1)	NL, IIEN, NET 3I4 Formats for next card	NL - number of expected energy levels with units of IIEN NET = 0 zero of potential at $R = \infty$ NET = 1 zero of potential at $R = R_e$
9+N(1)	KV(I, IKON), ETRIAL (I, IKON)	KV - the vibrational level ETRIAL - energy of the vibrational level KV(IKON) in number
(for upper state)		
10+N(1)	IIRA, IIEN, N(IKON) same	Same as for lower state
11+N(1)	XI, YI	Potential for upper state; same description as lower state N(2) in number
through		
11+N(1)+N(2)		
12+N(1) +N(2)	NDE, DE(IKON) Same	Same as for lower state
13+N(1) +N(2)	XMIN, XMAX, XH, IIRAI	Same as for lower state
14+N(1) +N(2)	NL (IKON) IIEN1, NET	Same as for lower state
15+N(1) +N(2)	KV (I, IKON) ETRIAL (I, IKON)	Same as for lower state
16+N(1) +N(2)	NI, NS, IPSIQ, MAXIT, EPS 4I4, E10.0	NI - 1 prints iterations, other- wise not

Card Number

Card 16 (cont'd)

		NS = 1 prints wavefunctions every IPSIQ points
		NS = 33 prints eigenvalues and node count
		MAXIT - maximum number of times SCHR will try and satisfy convergence criterion
		EPS - convergence criterion
17+N(1) +N(2)	JROTL, JROTU 2I3	lower and upper rotational levels respectively
18+N(1) +N(2)	BE1, AE1, GE1, BE2, AE2, GE2 6E10.3	rotational constants for lower and upper states
19+N(1) +N(2)	TE E10.3	TE - relative difference in energy (units of 1/cm) of the lower and upper states
20+N(1) +N(2)	NPOT I3	potential printed every NPOT points
21+N(1) +N(2)	Blank	

NOT REPRODUCIBLE

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PROGRAM FRANKLIN(INPUT,OUTPUT,PLUNCH)
C FRANKLIN CALCULATES VIBRATIONAL TRANSITION PROBABILITIES FOR
C DIATOMIC MOLECULES. IT IS BASED ON A PROGRAM OBTAINED FROM R.
C ZARE. THE POINTS DEFINING THE POTENTIAL ARE READ INTO THE PROGRAM
C A SPLINE FIT IS USED TO INTERPOLATE FROM THESE TO THE INTEGRATION
C GRID. THE INNER BRANCH OF THE POTENTIAL IS THEN EXTRAPOLATED BY A
C FUNCTION OF THE FORM A/R**F(R). THE OUTER BRANCH IS EXTRAPOLATED
C BY A FUNCTION OF THE FORM DE-A/R**F(R). THE SO DEFINED POTENTIAL
C IS USED IN THE SCHRODINGER EQUATION WHICH IS SOLVED BY SUBROUTINE
C SCHRO. THE WAVEFUNCTIONS ARE INTEGRATED BY MEANS OF A SIMPSON'S
C RULE SCHEME IN THE OVERLAP INTEGRAL.
C
C N=NUMBER OF POINTS DEFINING THE POTENTIAL,MUST BE 60 OR LESS
C NL=NUMBER OF LEVELS,MUST BE 30 OR LESS
C
COMMON X(6,1),Y(6,60),XO(10000),X(10000),S(10000),ETRIAL(30),OIRAL(
1),OIRN(3),OIRN(2),ZIRN(2),ZIRN(3),FCALC(30),YDRN(5),RVE(30
2),VPRN(5),OTRINT(10),OIENT(10),RVE(30),RESULT(30,30),PCNTRD(30,30)
3,RRCH(30,30),RRCH(30,30),RRCH(30,30),KV(30),N(2),NL(2),DE(2),PRE
4NT(10),PHET(10),DIV(50),SUMPR(30),SUMPR(30),TITLE(8),YH,NSTA,NSTA,M
5,XMIN,XMAX,INFC,MREQ,MUSED,NI,NS,MAXIT,FACH,ZMU,IKON,EDS,IP510,SCH
6R,SU(10000)
C DIMENSION XSTATE(2)
C
C THE FOLLOWING COMMENT CARDS DESCRIBE THE PREPARATION OF DATA.
C
C FIRST CARD IN DATA HAS A ONE IN COLUMN 1 IF A PROBLEM FOLLOWS.
C VERY LAST CARD IN DATA MUST BE A BLANK CARD.....
C
C INITIALIZING PLOT ROUTINE...
C
C NEXT CARD IN DATA HAS NAME OF PROBLEM IN COLUMNS 1-72, WHERE
C CARRIAGE CONTROL IS IN COLUMN 1. SECOND CARD HAS IIMS AND
C MASSES OF THE TWO ATOMS.
C IF ZMASS2 = 0, ZMASS1 IS TAKEN AS THE REDUCED MASS IN THE IIMS UNITS
C IIMS = 1, MASS UNITS ARE BASED ON O12 = 12.
C IIMS = 2, MASS UNITS ARE BASED ON O16 = 16.
C
C LIMIT ON N(IKON) IS 60, ON NL(IKON) IS 30 VIBRATIONAL LEVELS
1 READ 74, ITEST
C IF (ITEST) 2,75,2
C ICKTR = CHECK TO DETERMINE WHETHER WAVEFUNCTIONS WILL BE CALCULATED
C FOR OR READ FROM TAPE 1. ICKTR=0 FOR CALCULATION, ICKTR=1 READ FROM
C TAPE
2 READ 73, TITLE
C READ 74, ICKTR
C STATE(1) = 10 THE LOWER STATE, STATE(2) = 10 THE UPPER STATE
C READ 77, XSTATE(1)
C READ 77, XSTATE(2)
C READ 78, IIMS,ZMASS1,ZMASS2
C
C SET-UP FOR PLOTTING POTENTIALS...
C END OF PLOT SET-UP
C
C NEXT DATA CARD CONTAINS XMIN,XMAX,YH,IPRA, WHERE IPRA GIVES THE

```

C	UNITS FOR THE MIN AND MAX DISTANCES AND THE SPACING XH.	A	54
C	READ R0, XMINTEM, XMAXTEM, XHTEM, IIRA1	A	55
C	NEXT TWO CARDS ARE THE VALUES OF J FOR THE LOWER AND UPPER STATE	A	56
C	READ R1, JBOT, JTOT	A	57
C	NEXT CARD IN DATA HAS IIRA, IJEN, AND THE NUMBER OF POINTS, EACH	A	58
C	IN 14 FORMAT, AS WELL AS THE FORMAT STATEMENT WHICH CONTROLS THE	A	59
C	READING OF THE POINTS (IN COLUMNS 13-72)--FOR EXAMPLE- (4F16.8).	A	60
C	IJEN = 1, ENERGY IS IN ATOMIC UNITS. (1 A.U. = 27.1961 E.V.)	A	61
C	IJEN = 2, ENERGY IS IN 1/CM.	A	62
C	IJEN = 3, ENERGY IS IN ELECTRON VOLTS. (1 E.V. = 8065.68 1/CM)	A	63
C	IIRA = 1, DISTANCE IS IN ATOMIC UNITS. (1 A.U. = .529166 ANG.)	A	64
C	IIRA = 2, DISTANCE IS IN ANGSTROMS.	A	65
C	FOLLOWING CARDS CONTAIN THE INPUT POTENTIAL POINTS.	A	66
C	IF IT IS DESIRED TO USE A FUNCTION TO GENERATE THE WHOLE	A	67
C	POTENTIAL CURVE, THE FIRST 12 COLUMNS OF THE IIRA, ETC. CARD	A	68
C	MUST BE BLANK. A HOLLERITH TEXT MUST BE PUNCHED IN 13-72, AS	A	69
C	IT WILL BE PRINTED. THE NEXT CARD IN SUCH A CASE CONTAINS	A	70
C	XMIN, XMAX, ETC.	A	71
C	UPPER STATE IS READ IN FIRST, LOWER STATE LAST	A	72
C	THE SAME VALUE OF IJEN, IIRA, NDE, XH, XMIN, XMAX, IIRA1, NET	A	73
C	, IJEN1 MUST BE USED FOR BOTH THE GROUND AND UPPER STATE	A	74
C	IKON=2	A	75
3	READ R2, IIRA, IJEN, N(IKON), (DTERMT(I), I=1,10)	A	76
	XMIN=XMINTEM	A	77
	XMAX=XMAXTEM	A	78
	XH=XHTEM	A	79
	N(IKON)=N(IKON)	A	80
C	READ DTERMT, (XI(I), YI(I), I=1, N(IKON))	A	81
	NDO=N(IKON)/2	A	82
	NZD=NDO+1	A	83
	READ DTERMT, XI(NZD), YI(NZD), DDD, DDD1	A	84
	IM=IM=NZD	A	85
	DO 4 I=1, NDO	A	86
	IM=IM-1	A	87
	IM=IM+1	A	88
	READ DTERMT, XI(IM), YI(IM), YI(IM), YI(IM)	A	89
	YI(IM)=YI(IM)	A	90
4	CONTINUE	A	91
C	NEXT CARD CONTAINS NDE AND THE DISSOCIATION ENERGY WHERE NDE IS	A	92
C	ZERO IF ZERO PT OF POTENTIAL CURVE IS AT P=INFINITY, OR ONE IF AT	A	93
C	P=PEQUILIBRIUM. DISSOCIATION ENERGY HAS SAME UNITS AS POTENTIAL.	A	94
C	READ R3, NDE, DE(IKON)	A	95
C	NEXT CARD HAS NC, AND IJEN OF EXPECTED ENERGY LEVELS, AND NET	A	96
C	WHICH HAS THE SAME INTERPRETATION FOR ETIPAL(I) AS NDE DOES FOR	A	97
C	THE POTENTIAL CURVE ABOVE.	A	98
C	IT ALSO CONTAINS THE VARIABLE FORMAT FOR READING ENERGY LEVELS	A	99
C		A	100

```

C      READ R4, NLIKON, IIFN1, NFX, (DUEMT(I), I=1, 10)
C      NLIKON=N(IKON)
C      READ IN ENERGY LEVELS
C      READ DUEMT, (KV(I), ETRIAL(I), I=1, NLIKON)
C      READ IN THE EXPERIMENTAL RV, CALLED RVE
C      READ R5, (RVE(I), I=1, NLIKON)
C      DOING FIRST FOR THE UPPER STATE AND THEN THE LOWER STATE, SCHRODING
C      EPS EQUATION USING THE FOLLOWING METHOD
C      D2 NL SCHR MODIFIED FOR THE 700/7000/7004 IS DESCRIBED IN
C      P. N. ZARE AND J. V. CASHION, UCRL-10881, 1963
C      FOR THIS PROGRAM THE CONSTANTS ARE USED AS FOLLOWS
C      IF NI = 1, PRINTS ITERATIONS, OTHERWISE NOT
C      IF NS = 1, PRINTS WAVEFUNCTION EVERY 1000 POINTS, OTHERWISE NOT
C      IF NS = 33, PRINTS EIGENVALUES AND MODE COUNT
C      EPS IS THE CONVERGENCE CRITERION
C      EPS IS IN THE SAME UNITS AS THE POTENTIAL CURVE
C      MAXIT IS THE MAXIMUM NUMBER OF TIMES SCHR WILL TRY TO SATISFY THE
C      CONVERGENCE CRITERION
C
C      LLIM=100
C      KLLIM=2
C      READ R6, NI, NS, ITRISIO, MAXIT, EPS
C
C      NEXT CARD CONTAINS NPOT,
C      THE POTENTIAL IS PRINTED AT EVERY NPOT POINT,
C      NPOT = 50 IS SUGGESTED TO THE USER.
C
C      READ R1, NPOT
C
C      THIS TERMINATES COMMENT CARDS ON THE PREPARATION OF DATA.
C      IF NO FURTHER PROBLEMS FOLLOW, REMEMBER TO ADD A BLANK CARD TO THE
C      DATA DECK
C
C      QIPA(1)=6.44A.U.
C      QIPA(2)=6.44ANGST.
C      QIFN(1)=6.44A.U.
C      QIFN(2)=6.44/CM
C      QIFN(3)=6.44E.V.
C      QIMS(1)=6.44E12=12
C      QIMS(2)=6.44E16=16
C
C      OUTPUT IS IN WAVE NUMBERS AND ANGSTROMS
C      PRINT HEADING
C
C      PRINT 70, TITLE
C
C      PRINT R1, JDOT1, JDOT2
C      PRINT THE MASSES AND THEIR UNITS.
C
C      IF (ZNACT) 6.44E

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5	PRINT 87, QIMS(IIMS),ZMAS1,ZMAS2	A 166
	GO TO 7	A 167
6	PRINT 88, QIMS(IIMS),ZMAS1	A 168
7	CONTINUE	A 169
C		A 170
C	PRINT THE INPUT POTENTIAL, THE DISSOCIATION ENERGY, AND UNITS.	A 171
C	IF READ IN,	A 172
C		A 173
	PRINT 89, QIPA(IIRA),QIFN(IIFN)	A 174
	NIKON=N(IKON)	A 175
	PRINT 90, (XI(I),YI(I),I=1,NIKON)	A 176
	PRINT 91, DE(IKON)	A 177
	PRINT 92, YMIN,XMAX,XH,QIPA(IIRA1)	A 178
C		A 179
C	PRINT THE TRIAL ENERGY LEVELS AND THEIR UNITS.	A 180
C		A 181
	PRINT 93, QIFN(IIFN1),(KV(I),ETRIAL(I),I=1,NLIKON)	A 182
C		A 183
C	PRINT THE CONVERGENCE CRITERION.	A 184
C		A 185
	PRINT 94, EPS,QIFN(IIFN)	A 186
C		A 187
C	PRINT HEADING	A 188
	PRINT 95, TITLE	A 189
C	PLOTTING GENERATED POTENTIALS...	A 190
C		A 191
	IF (ZMAS2) R,R,0	A 192
8	ZMU=ZMAS1	A 193
	GO TO 10	A 194
9	ZMU=ZMAS1+ZMAS2/(ZMAS1+ZMAS2)	A 195
10	ZIMS(1)=1.0	A 196
	ZIMS(2)=.0006784	A 197
	ZIRA(1)=1.0	A 198
	ZIRA(2)=1.889766	A 199
	ZMU=ZMU*ZIMS(IIMS)	A 200
	ZIFN(1)=ZMU*3.643668E2	A 201
	ZIFN(2)=ZMU*1.6610826E-2	A 202
	ZIFN(3)=ZMU*1.330776E2	A 203
	EACH=60.201702/ZMU	A 204
	N2=N(2)	A 205
	NL2=NL(2)	A 206
	IND=N(IKON)	A 207
	DO 11 I=1,IND	A 208
	YI(I)=YI(I)*ZIFN(IIFN)	A 209
	YI(I)=YI(I)*ZIRA(IIRA)	A 210
11	CONTINUE	A 211
	DE=DE*ZIFN(IIFN)	A 212
	DE(2)=DE(2)*ZIFN(IIFN)	A 213
	YMIN=XMIN*ZIRA(IIRA1)	A 214
	YMAX=YMAX*ZIRA(IIRA1)	A 215
	XH=XH*ZIRA(IIRA1)	A 216
	EPS=EPS*ZIFN(IIFN)	A 217
	INDL=NL(IKON)	A 218
	DO 12 I=1,INDL	A 219
	ETRIAL(I)=ETRIAL(I)*ZIFN(IIFN1)	A 220

12	CONTINUE	A 221
	CALL POTFIT	A 222
C	CHECK FOR RESCALING OF POTENTIAL TO ZERO AT R=INFINITY	A 223
	IF (INDE) 74,15,13	A 224
13	DO 14 I=1,M	A 225
	V(I)=V(I)-DE(IKON)	A 226
14	CONTINUE	A 227
15	IF (MET) 71,18,16	A 228
16	DO 17 I=1,INDL	A 229
	ETRIAL(I)=ETRIAL(I)-DE(IKON)	A 230
17	CONTINUE	A 231
18	DO 19 I=1,INDL	A 232
	FCALC(I)=ETRIAL(I)	A 233
19	CONTINUE	A 234
C		A 235
C	PRINT THE POTENTIAL CURVE GENERATED (ANGSTROMS AND 1/CM)	A 236
C	272 WRITE(1),ISTATE,IKON,M	A 237
C	RUFFER OUT(1,1)(XO(1),XO(M))	A 238
C	135 CONTINUE	A 239
C	IF (UNIT,1) 135,240,240,240	A 240
C	240 RUFFER OUT(1,1)(V(1),V(M))	A 241
	PRINT 95	A 242
	NPOT4=NPOT*4	A 243
	NPOT5=NPOT*5	A 244
	DO 26 I=1,M,NPOT5	A 245
	IF (M-I-NPOT4) 20,21,21	A 246
20	JFIN=(M-I)/NPOT	A 247
	IF (JFIN) 27,27,22	A 248
21	JFIN=5	A 249
22	DO 23 J=1,JFIN	A 250
	IPRN=I+NPOT*(J-1)	A 251
	XPRN(J)=XO(IPRN)*.529146	A 252
	VPRN(J)=(V(IPRN)+DE(IKON))*FACM	A 253
23	CONTINUE	A 254
	IF (VPRN(1)-1,F6) 25,24,24	A 255
24	PRINT 96, (XPRN(J),VPRN(J),J=1,JFIN),IPRN	A 256
	GO TO 26	A 257
25	PRINT 97, (XPRN(J),VPRN(J),J=1,JFIN),IPRN	A 258
26	CONTINUE	A 259
27	MTEMQ=M	A 260
	LLK=0	A 261
	FLK=0	A 262
C	FIND THE ENERGY LEVELS THROUGH USE OF SCHR.	A 263
	DO 40 I=1,MLIKON	A 264
	CALL SCHR0 (KV(I),FCALC(I))	A 265
	IF (SCHR-1.) 29,28,71	A 266
28	LLY=LLK+1	A 267
	IF (LLK=LLTY) 29,29,73	A 268
29	M=MTEMQ	A 269
	DO 30 J=1,M	A 270
30	XO(J)=(J-1)*XH+XMIN	A 271
	RVSIJM=S(1)**2/XO(1)**2+4.*S(2)**2/XO(2)**2+S(M)**2/XO(M)**2	A 272
	VSIMP=M-1	A 273
	DO 31 J=2,VSIMP,2	A 274
	RVSIJM=2.*S(J)**2/XO(J)**2+4.*S(J+1)**2/XO(J+1)**2+RVSIJM	A 275

31	CONTINUE	A 276
C	ALSO WRITE WAVEFUNCTION ONTO TAPE	A 277
C	WRITE(1)IKON,NLIKON,I,M	A 278
C	IKON=POTENTIAL,NLIKON=NUMBER OF VIBRATIONAL LEVELS FOR	A 279
C	POTENTIAL IKON,I=NUMBER OF THE LEVEL,M=NUMBER OF POINTS AT WHICH	A 280
C	WAVEFUNCTION IS TABULATED	A 281
C	BUFFER OUT (1,1)(S(1),S(M))	A 282
C	GO TO (33,22), IKON	A 283
C	PUT WAVEFUNCTION INTO EXTENDED CORE FOR LATER USE	A 284
32	INFC=1+(I-1)*M	A 285
	CALL WRITEC (S(1),INFC,M)	A 286
	GO TO 30	A 287
33	DO 38 IK=1,NL2	A 288
	INFC=1+M*(IK-1)	A 289
	CALL READFC (SU(1),INFC,M)	A 290
	DO 34 J=1,M	A 291
	XO(J)=(FLOATE(J-1)*XH+XM*IN)*SU(J)	A 292
34	CONTINUE	A 293
	CALL SIMP (S,SU,M,XH,RESULT(I,IK))	A 294
	CALL SIMP (S,XO,M,XH,PCNTPD(I,IK))	A 295
	A=XM*IN	A 296
	DO 35 J=1,M	A 297
	YO(J)=A*XO(J)	A 298
	A=A+XH	A 299
35	CONTINUE	A 300
	CALL SIMP (S,XO,M,XH,PCN(I,IK))	A 301
	A=XM*IN	A 302
	DO 36 J=1,M	A 303
	XO(J)=A*XO(J)	A 304
	A=A+XH	A 305
36	CONTINUE	A 306
	CALL SIMP (S,XO,M,XH,PPRCN(I,IK))	A 307
	A=XM*IN	A 308
	DO 37 J=1,M	A 309
	XO(J)=A*XO(J)	A 310
	A=A+XH	A 311
37	CONTINUE	A 312
	CALL SIMP (S,XO,M,YH,PPPRN(I,IK))	A 313
38	CONTINUE	A 314
39	RVE(I)=FACM*RVSIM*XH/3.	A 315
	FCALC(I)=DE(IKON)*FACM+FCALC(I)	A 316
	PRINT 98, FCALC(I),RVE(I)	A 317
40	CONTINUE	A 318
	PRINT 78, TITLE	A 319
	PRINT 99, LLK	A 320
	PRINT 100, XSTATE(IKON)	A 321
	PRINT 101	A 322
	DO 42 I=1,NLIKON	A 323
	ETRIAL(I)=(ETRIAL(I)+DE(IKON))*FACM	A 324
	DIEF=FCALC(I)-ETRIAL(I)	A 325
	IF (I-1) 42,42,41	A 326
41	DGT=ETRIAL(I)-ETRIAL(I-1)	A 327
	DGC=FCALC(I)-FCALC(I-1)	A 328
	DIEDE=DGC-DGT	A 329
	PRINT 102, DGT,DGC,DIEDE	A 330

42	PRINT 103, KV(1),ETRIAL(1),FCALC(1),DIFF	A 231
43	CONTINUE	A 232
	PRINT 104, XSTATE(IKON)	A 233
	PRINT 105	A 234
	DO 44 I=1,NI IKON	A 235
	PRINT 106, KV(1),PVE(1),PVE(1)	A 236
44	CONTINUE	A 237
	GO TO (46,45), IKON	A 238
45	IKON=1	A 239
	GO TO 3	A 240
46	CONTINUE	A 241
	DO 47 J=1,NI	A 242
	DO 47 IK=1,NI 2	A 243
	DEF=RESULT(J,IK)	A 244
	R=0.520166	A 245
	PCNTRD(J,IK)=PCNTRD(J,IK)*R/DEF	A 246
	R=R*0.520166	A 247
	PRCN(J,IK)=PRCN(J,IK)*R/DEF	A 248
	R=R*0.520166	A 249
	PRRCN(J,IK)=PRRCN(J,IK)*R/DEF	A 250
	R=R*0.520166	A 251
	PRRPN(J,IK)=PRRPN(J,IK)*R/DEF	A 252
	RESULT(J,IK)=DEF*DEF	A 253
47	CONTINUE	A 254
	PRINT 107, TITLE	A 255
	NLIS=15NLIF=10	A 256
48	CONTINUE	A 257
	PRINT 109, (KV(J),J=NLIS,NLIF)	A 258
	DO 49 J=1,NL2	A 259
	K=J-1	A 260
	PRINT 108, K, (DEFULT(ILK,J),ILK=NLIS,NLIF)	A 261
	IF (MOD(J,5).NE.0) GO TO 49	A 262
	PRINT 114	A 263
49	CONTINUE	A 264
	PRINT 115	A 265
	IF (NLIF.GE.NL) GO TO 50	A 266
	NLIS=NLIF+15NLIF=NLIS+0	A 267
	IF (NLIF.LT.NL) GO TO 48	A 268
	NLIF=NL5GOTO27	A 269
50	CONTINUE	A 270
C	SUMMING FCF	A 271
	DO 51 J=1,NI	A 272
	DO 51 JJ=1,NL2	A 273
51	SUMPD(J)=SUMPD(J)+RESULT(J,JJ)	A 274
	DO 52 JJ=1,NL2	A 275
	DO 52 J=1,NI	A 276
52	SUMP(JJ)=SUMP(JJ)+DEFULT(J,JJ)	A 277
	PRINT 108, TITLE	A 278
	DO 53 J=1,NI	A 279
	JM1=J-1	A 280
	PRINT 110, JM1,SUMPD(J)	A 281
53	SUMPD(J)=0.	A 282
	DO 54 JJ=1,NL2	A 283
	JJM1=JJ-1	A 284
	PRINT 111, JJM1,SUMP(JJ)	A 285

54	SUMD(JJ)=0. PRINT 112, TITLE NLIS=1\$NLIF=14	A 386 A 387 A 388
55	CONTINUE PRINT 127, (KV(J),J=NLIS,NLIF) DO 56 J=1,NL2 K=J-1	A 389 A 390 A 391 A 392
	PRINT 113, K, (PCNTRD(ILK,J),ILK=NLIS,NLIF) IF (MOD(J,5).NE.0) GO TO 56 PRINT 114	A 393 A 394 A 395
56	CONTINUE PRINT 115 IF (NLIF.GE.NL) GO TO 57 NLIS=NLIF+1\$NLIF=NLIS+12 IF (NLIF.LT.NL) GO TO 55 NLIF=NL\$GOTO6001	A 396 A 397 A 398 A 399 A 400 A 401
57	CONTINUE PRINT 116, TITLE NLIS=1\$NLIF=14	A 402 A 403 A 404
58	CONTINUE PRINT 127, (KV(J),J=NLIS,NLIF) DO 59 J=1,NL2 K=J-1	A 405 A 406 A 407 A 408
	PRINT 113, K, (PRCN(ILK,J),ILK=NLIS,NLIF) IF (MOD(J,5).NE.0) GO TO 59 PRINT 114	A 409 A 410 A 411
59	CONTINUE PRINT 115 IF (NLIF.GE.NL) GO TO 60 NLIS=NLIF+1\$NLIF=NLIS+12 IF (NLIF.LT.NL) GO TO 58 NLIF=NL\$GOTO6002	A 412 A 413 A 414 A 415 A 416 A 417
60	CONTINUE PRINT 117, TITLE NLIS=1\$NLIF=14	A 418 A 419 A 420
61	CONTINUE PRINT 127, (KV(J),J=NLIS,NLIF) DO 62 J=1,NL2 K=J-1	A 421 A 422 A 423 A 424
	PRINT 113, K, (PRRCN(ILK,J),ILK=NLIS,NLIF) IF (MOD(J,5).NE.0) GO TO 62 PRINT 114	A 425 A 426 A 427
62	CONTINUE PRINT 115 IF (NLIF.GE.NL) GO TO 63 NLIS=NLIF+1\$NLIF=NLIS+12 IF (NLIF.LT.NL) GO TO 61 NLIF=NL\$GOTO651	A 428 A 429 A 430 A 431 A 432 A 433
63	CONTINUE PRINT 118, TITLE NLIS=1\$NLIF=14	A 434 A 435 A 436
64	CONTINUE PRINT 127, (KV(J),J=NLIS,NLIF) DO 65 J=1,NL2 K=J-1	A 437 A 438 A 439 A 440

	PRINT 113, K, (PPDRN(ILK,J),ILK=NLIS,NLIF)	A 441
	IF (MOD(J,5).NE.0) GO TO 65	A 442
	PRINT 114	A 443
65	CONTINUE	A 444
	PRINT 115	A 445
	IF (NLIF.GE.NL) GO TO 66	A 446
	NLIS=NLIF+15NLIF=NLIS+13	A 447
	IF (NLIF.LT.NL) GO TO 64	A 448
	NLIF=NLISGOTO555	A 449
66	CONTINUE	A 450
	PUNCH 119, TITLE	A 451
	PUNCH 121, NL2,NL	A 452
	PUNCH 122	A 453
	PUNCH 123, ((I,J,RESULT(J,I),J=1,NL),I=1,NL2)	A 454
	PUNCH 123	A 455
	PUNCH 124, ((I,J,RCNTRD(J,I),J=1,NL),I=1,NL2)	A 456
	PUNCH 125	A 457
	PUNCH 124, ((I,J,RPCN(J,I),J=1,NL),I=1,NL2)	A 458
	PUNCH 126	A 459
	PUNCH 124, ((I,J,RRRCN(J,I),J=1,NL),I=1,NL2)	A 460
	DO 67 IK=1,NL2	A 461
	DO 67 J=1,NL	A 462
	RESULT(J,IK)=RCNTRD(J,IK)/RPCN(J,IK)	A 463
	RCNTRD(J,IK)=RPCN(J,IK)/RRRCN(J,IK)	A 464
	RRCN(J,IK)=PPPCN(J,IK)/RRRCN(J,IK)	A 465
67	CONTINUE	A 466
	PRINT 128, TITLE	A 467
	NLIS=15NLIF=14	A 468
68	CONTINUE	A 469
	PRINT 127, (KV(J),J=NLIS,NLIF)	A 470
	DO 69 J=1,NL2	A 471
	K=J-1	A 472
	PRINT 129, (RESULT(J,ILK),ILK=NLIS,NLIF)	A 473
	PRINT 130, K, (PCNTRD(J,ILK),ILK=NLIS,NLIF)	A 474
	PRINT 131, (RPCN(J,ILK),ILK=NLIS,NLIF)	A 475
	IF (MOD(J,5).NE.0) GO TO 69	A 476
	PRINT 114	A 477
69	CONTINUE	A 478
	PRINT 115	A 479
	IF (NLIF.GE.NL) GO TO 70	A 480
	NLIS=NLIF+15NLIF=NLIS+13	A 481
	IF (NLIF.LT.NL) GO TO 68	A 482
	NLIF=NLISGOTO601	A 483
70	CONTINUE	A 484
	GO TO 1	A 485
71	KLK=KLK+1	A 486
	IF (KLK=KLIM) 20,72,72	A 487
72	PRINT 132, KLIM	A 488
	GO TO 1	A 489
73	PRINT 133, LLIM,I	A 490
	GO TO 1	A 491
74	PRINT 6, NDE	A 492
	GO TO 1	A 493
75	CALL EXIT	A 494
C		A 495

76	FORMAT (I1)	A 496
77	FORMAT (A10)	A 497
78	FORMAT (8A10)	A 498
79	FORMAT (14.2F10.0)	A 499
80	FORMAT (2F10.0,I4)	A 500
81	FORMAT (2I3)	A 501
82	FORMAT (3I4,10A6)	A 502
83	FORMAT (14,F10.0)	A 503
84	FORMAT (3I4,10A6)	A 504
85	FORMAT (8F10.0)	A 505
86	FORMAT (4I4,F10.0)	A 506
87	FORMAT (///40H THE MASSES OF THE TWO ATOMS, BASED ON A6.6H, ARE F	A 507
	110.6.5H AND F10.6.6///)	A 508
88	FORMAT (///46H THE REDUCED MASS OF THE TWO ATOMS, BASED ON A6.5H,	A 509
	1 IS F10.6.6///)	A 510
89	FORMAT (35H THE INPUT POTENTIAL POINTS, R IN A6.15H AND ENERGY IN	A 511
	1 A6.18HARE GIVEN BELOW. //1X.5(6X.1HR.10X.1HV.4X)///)	A 512
90	FORMAT (1XF10.6,F12.4,F10.6,F12.4,F10.6,F12.4,F10.6,F12.4,F10.6,F1	A 513
	12.4)	A 514
91	FORMAT (47H0 DISSOCIATION ENERGY IN SAME UNITS AS ABOVE ISE20.8)	A 515
92	FORMAT (////20H RMIN = F10.7.0H, RMAX = F10.7.12H, SPACING = F10.7	A 516
	1.0H, ALL IN A6)	A 517
93	FORMAT (////20H THE TRIAL ENERGY LEVELS IN A6.16HARE GIVEN BELOW.	A 518
	1//1X.5(5HLEVEL.3X.6HENERGY.6X)///(1H I4.1PF16.7.I4.F16.7I4.F16.7.I4	A 519
	2.F16.7.I4.F16.7))	A 520
94	FORMAT (////43H CONVERGENCE CRITERION IS ERROR LESS THAN E9.2.2XA	A 521
	14)	A 522
95	FORMAT (37H0 THE POTENTIAL FUNCTION GENERATED IS///1X.5(3X.4HR(A).	A 523
	14X.7HV(1/CM)2X))	A 524
96	FORMAT (1X0PF10.6,1PF12.5,4(0PF10.6,1PF12.5),4X15)	A 525
97	FORMAT (1XF10.6,F12.4,F10.6,F12.4,F10.6,F12.4,F10.6,F12.4,F10.6,F1	A 526
	12.4,4X15)	A 527
98	FORMAT (30H0 SCHR FINDS ENERGY LEVEL G = F11.5.15H 1/CM AND RV = F	A 528
	111.7.5H 1/CM)	A 529
99	FORMAT (38H0 PROGRAM SUCCESSFUL. (MAXIT REACHED 12.7H TIMES))	A 530
100	FORMAT (23H0 THE BELOW IS FOR THE STATE A10)	A 531
101	FORMAT (54H0VIR. NO. GIVEN ENERGY CALC. ENERGY DIFFERENCE1	A 532
	13X.43H GIVEN DELTA G CALC. DELTA G DIFFERENCE/44X.26H0DIFFERENC	A 533
	2F = CALC. - GIVEN//)	A 534
102	FORMAT (64X7F15.5)	A 535
103	FORMAT (18.7F15.5)	A 536
104	FORMAT (20H1 THE BELOW IS FOR THE STATE A10)	A 537
105	FORMAT (14028X.8HV10. NO.,3X.0H0CALC. RV5X.0H0EXP. RV ///)	A 538
106	FORMAT (28X17.7F15.5)	A 539
107	FORMAT (28H1 FRANCK CONDN FACTORS FOR .8A10)	A 540
108	FORMAT (13.1X.10(2X.F10.3))	A 541
109	FORMAT (1H .2X.4HV.0.4X.10(12.10X)/1X.2HV.//)	A 542
110	FORMAT (20H THE SUM OVER ALL V-- FOR V--=.13.2H15.F12.8)	A 543
111	FORMAT (20H THE SUM OVER ALL V-- FOR V--=.13.2H15.F12.8)	A 544
112	FORMAT (37H1 D CENTROID FACTORS (ANGSTROMS) FOR .8A10)	A 545
113	FORMAT (14.14(3X.F6.4))	A 546
114	FORMAT (1H)	A 547
115	FORMAT (1H ///)	A 548
116	FORMAT (20H1 P**2 CENTROIDS FOR .8A10)	A 549
117	FORMAT (20H1 P**3 CENTROIDS FOR .8A10)	A 550

118	FORMAT (19H) R**4 CENTROID FOR.8A10)	A 551
119	FORMAT (8A10)	A 552
120	FORMAT (23H FRANCK CONDON FACTORS)	A 553
121	FORMAT (213)	A 554
122	FORMAT (4(213,2X,F12.5))	A 555
123	FORMAT (13H P CENTROIDS)	A 556
124	FORMAT (6(1X,212,F8.4))	A 557
125	FORMAT (16H R**2 CENTROIDS)	A 558
126	FORMAT (16H R**3 CENTROIDS)	A 559
127	FORMAT (1H0,3X,3HVV=.3X,14(12.7X)/2X,1HV/)	A 560
128	FORMAT (24H1 RATIO OF CENTROIDS FOR.8A10)	A 561
129	FORMAT (1H,4X,14(3X,F6.4))	A 562
130	FORMAT (1H,12,4X,14(3X,F6.4))	A 563
131	FORMAT (1H,8X,14(3X,F6.4))	A 564
132	FORMAT (26H0 SCHR NOT SUCCESSFUL FOR 12.28HTH TIME, GO TO NEXT PRO BLEM.)	A 565
133	FORMAT (28H0 SCHR DID NOT CONVERGE FOR 12.17HTH TIME WHEN I = 13)	A 567
	END	A 568-

	SUBROUTINE POTFIT	R	1
	COMMON XI(60),YI(60),XO(10000),VO(10000),S(10000),ETRIAL(30),QIRA(2	R	2
	1),QIFN(3),QIMS(2),ZIMS(2),ZIRA(2),ZIFN(3),FCALC(30),XPRN(5),BVF(30	R	3
	2),VPRN(5),DTERMT(10),DUFMT(10),BVF(30),RESULT(30,30),RCNTRD(30,30)	R	4
	3,RRCN(30,30),RPRCN(30,30),RRRRN(30,30),KV(30),N(2),NL(2),DE(2),PRF	R	5
	4MT(10),PNET(10),DIV(50),SUMPP(30),SUMP(30),TITLE(8),XH,NSTA,MSTA,M	R	6
	5,XMIN,XMAX,INSC,MREG,MUSED,NI,NS,MAXIT,FACH,ZMU,IKON,EPS,PSIQ,SCH	R	7
	60,SU(10000)	R	8
	DIMENSION Z(60),AX(60),PY(60),CX(60),DX(60)	R	9
	YMAXT=XMAX	R	10
	YMINI=YMIN	R	11
C	CHECK FOR EXTRAPOLATION AT SMALL P.	R	12
	IF (XMIN-XI(1)) 1,2,2	R	13
1	XMAX=XI(1)	R	14
	INSC=1	R	15
	NLL=N(1KON)	R	16
	CALL XTPAD (XI,YI,NLL,XO,V,M,XH,XMIN,XMAX,INSC,FACH,MREG,DE(1KON))	R	17
	MT=M	R	18
	YMIN=XO(MT)+XH	R	19
	MREG=M+1	R	20
C	PREPARE TO INTERPOLATE.	R	21
2	M=0	R	22
	XMAX=XMAXT	R	23
	IF (XMAX-XI(NLL)) 4,4,3	R	24
3	XMAX=XI(NLL)	R	25
4	CALL SPLXYZ (XI,YI,2,NLL,AX,PY,CX,DX)	R	26
	MEND=MREG+INT((XMAX-XMIN)/XH)	R	27
	XOO=XMIN	R	28
	DO 5 II=MREG,MEND	R	29
	CALL SPNXYZ (XI,YI,2,NLL,XOO,VO)	R	30
	V(II)=VO	R	31
	XO(II)=XOO	R	32
5	XOO=XOO+XH	R	33
C	CHECK FOR EXTRAPOLATION AT LARGE P.	R	34
	IF (YMAXT-YMAX) 7,7,6	R	35
6	MREG=MEND+1	R	36
	XMIN=XO(MREG-1)+XH	R	37
	XMAX=YMAXT	R	38
	INSC=2	R	39
	CALL XTPAD (XI,YI,NLL,XO,V,M,XH,XMIN,XMAX,INSC,FACH,MREG,DE(1KON))	R	40
	INSC=0	R	41
7	YMIN=YMINI	R	42
	M=M+MREG-1	R	43
	RETURN	R	44
	END	R	45-


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SUBROUTINE SPXYV7 (Y,V,Z,N,UX,UY)
DIMENSION Y(1), V(1), Z(1)
DATA X6A/0.171552525252525252/
IF (UX-X(1)) 1,2,3
PRINT 13, UX,X(1),V(N),N
STOP 311
2 UY=V(1)
RETURN
3 IF (UY-X(N)) 5,4,1
4 UY=V(N)
RETURN
5 SH=N
SL=1.
6 I=(SH+SL)*.5
IF (UX-Y(I)) 7,11,10
7 SH=I
8 IF (SH-SL-.1) 9,12,6
9 STOP 312
10 SL=I
GO TO 8
11 UY=V(I)
RETURN
12 M=SL
MA=SH
YA=X(MA)-X(1)
YAA=YA*YA
XAB=1./XA
YB=X(MA)-UY
YBA=YB*YB
YBB=YB*(YBA-YAA)
YC=UY-X(1)
YCA=YC*YC
YCC=YC*(YCA-YAA)
UY=(1/2*(YBB+2*(MA)*YCC)+Y6A+(Y(MA)*YC+Y(N)*YB))*XAB
RETURN
C
13 FORMAT (1H1,1X,2F25.15,115)
END

```

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38
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	SUBROUTINE XTRAP (XI,YI,N,XO,V,M,XH,XMIN,YMAX,INSC,FACH,MREG,DF)	F	1
	DIMENSION XI(1), YI(1), XO(1), V(1), EN(2), XL(6), YL(6), SIGH(1),	F	2
	1 ANS(4)	F	3
C	V=C1*D** (A*LOG(D)+B)	F	4
	DF(X)=C1*X** (A*ALOG(X)+B)	F	5
	DF1(X)=DF-DF(X)	F	6
	IF (INSC.GT.1) GO TO 2	F	7
C	INITIALIZING SECTION FOR INNER BRANCH OF POTENTIAL	F	8
	M=XF1XF((XMAX-XMIN)/XH)+1	F	9
	MP=1	F	10
	IST=1	F	11
	IFIN=M	F	12
C	LEAST SQUARES PARAMETERS	F	13
	ILS=15 ILF=6	F	14
	DO 1 I=ILS,ILF	F	15
	XL(I)=ALOG(XI(I))	F	16
1	YL(I)=ALOG(YI(I))	F	17
	MPTS=65 NORDER=2 NINT=1	F	18
	SIGH(1)=XL(MPTS)	F	19
	CALL LSOPRT (XL,YL,NINT,NORDER,MPTS,SIGH,ANS)	F	20
	A=0.	F	21
	B=ANS(2)	F	22
	GO TO 4	F	23
C	INITIALIZING SECTION FOR OUTER BRANCH OF POTENTIAL	F	24
2	M=XF1XF((XMAX-XMIN)/YH)+1	F	25
	IFIN=MREG+M-1	F	26
	IST=MREG	F	27
	MP=M	F	28
C	SET UP LEAST SQUARES PARAMETERS	F	29
	ILS=N-5 ILF=M	F	30
C	FINDING A, B BY LEAST SQUARES METHOD FROM LAST 6 POINTS OF POTENT	F	31
	J=1	F	32
	DO 3 I=ILS,ILF	F	33
	YL(J)=ALOG(XI(I))	F	34
	YL(J)=ALOG(YI(I))	F	35
3	J=J+1	F	36
	MPTS=6	F	37
	NORDER=2	F	38
	NINT=1	F	39
	SIGH(1)=XL(MPTS)	F	40
	CALL LSOPRT (XL,YL,NINT,NORDER,MPTS,SIGH,ANS)	F	41
	A=0.	F	42
	B=-ANS(2)	F	43
C	C=ANS(1) BUT NOT USED	F	44
4	CONTINUE	F	45
	D1D=A*ALOG(XI(MD))*0.529166)+B	F	46
	D1=A*ALOG(YI(MD))+B	F	47
	IF (INSC.GT.1) GO TO 5	F	48
	C1=YI(MD)/XI(MD)**D1	F	49
	GO TO 6	F	50
5	C1=(DF-YI(MD))/XI(MD)**D1	F	51
6	CONTINUE	F	52
	DO 9 I=IST,IFIN	F	53
	XO(I)=FLOATE(I-IST)*XH+XMIN	F	54
	IF (INSC.GT.1) GO TO 7	F	55

	V(I)=PE(YO(I))	F	56
	GO TO 8	F	57
7	V(I)=PE(YO(I))	F	58
8	CONTINUE	F	59
9	CONTINUE	F	60
C	PRINT VARIABLE	F	61
	C1=C1*EACH*.520166**D1D	F	62
	EN(2)=5HRIGHT	F	63
	EN(1)=5HLEFT	F	64
	PRINT 10, EN(1)NSC)	F	65
	PRINT 11, A,B,C1,D1D	F	66
	RETURN	F	67
C		F	68
10	FORMAT (////40H THE PARAMETERS USED TO EXTRAPOLATE THE A5.46H BRANC	E	69
	1H OF THE POTENTIAL CURVE ARE AS FOLLOWS /)	E	70
11	FORMAT (3H A=E10.3,3H B=E10.3,4H C1=E10.3,4H D1=E10.3,32H WHERE V=	F	71
	1C1*X**D1, D1=A*LOG(Y)+B//)	F	72
	END	F	73-

	SUBROUTINE SCHRO (KV,EO)	F	1
C	NOTE COMMON NAMES HAVE BEEN CHANGED TO MAKE BLOCK COMPATABLE	F	2
C	WITH THIS SUBROUTINE	F	3
	COMMON XI(60),YI(60),XO(10000),V(10000),S(10000),ETRIAL(30),QIRA(2	F	4
	1),QIEN(3),QINS(2),ZIMS(2),ZIRA(2),ZIEN(3),ECALC(30),XPRN(5),RVE(30	F	5
	2),VPRN(5),DIERMT(10),DUFMT(10),RVE(30),RESULT(30,30),RCNTRD(30,30)	F	6
	3,RRCN(30,30),RRRCH(30,30),RRRRN(30,30),TV(30),L(2),NN(2),DD(2),PRE	F	7
	4MT(10),PNET(10),DIV(50),SUMPP(30),SUMP(30),TITLE(8),XH,NSTA,MSTA,N	F	8
	5,XMIN,XMAX,INSC,MREG,MUSED,NI,NS,MAXIT,FACM,ZMU,IKON,EPS,IPSIQ,SCH	F	9
	6P,SU(10000)	F	10
	DIMENSION Y(3), P(10000)	F	11
	EQUIVALENCE (P,XO), (YMIN,PMIN), (YMAX,RMAX)	F	12
C	SCHRV PRINTS EVERY IPSIQTH POINT OF THE WAVE FUNCTIONS.	F	13
C	RADIAL SOLUTION TO SCHRODINGER EQUATION SUBROUTINE	F	14
C	USE UNITS SUCH THAT SCHR EQN IS-PSI ² + (E-V)PSI = 0	F	15
C	NI=1, PRINT ITERATIONS	F	16
C	NI=OTHERWISE, DONT PRINT	F	17
C	NS=1, PRINT SOLUTIONS WITH EACH ENERGY LEVEL	F	18
C	NS=33, PRINT ENERGY LEVELS ONLY	F	19
C	NS=OTHERWISE, DONT PRINT	F	20
	IF (NI-1) 2,1,2	F	21
1	EPRIN=EO*FACM	F	22
	PRINT 42, KV,EPRIN	F	23
	PRINT 43	F	24
2	CONTINUE	F	25
	H=(RMAX-PMIN)/FLOAT(N-1)	F	26
	H2=H**2	F	27
	HV=H2/12.	F	28
	E=EO	F	29
	TEST=-1.	F	30
	DE=0.	F	31
C		F	32
C	START ITER LOOP	F	33
C		F	34
	DO 22 IT=1,MAXIT	F	35
CSTART INWARD INTEGRATION	F	36
	D(N)=1,E=EO	F	37
	GN=V(N)-E	F	38
	G1=V(N-1)-E	F	39
CTEST IF E TOO HIGH	F	40
	IF (G1) 3,4,4	F	41
3	PRINT 44	F	42
	SCHD=2.	F	43
	GO TO 41	F	44
4	D(N-1)=D(N)*EXP((PMAX*SORTE(GN)-(PMAX-H)*SORTE(G1))	F	45
	Y=(1.-HV*GN)*D(N)	F	46
	Y(2)=(1.-HV*G1)*D(N-1)	F	47
CINTEGRATE	F	48
	M=N-2	F	49
5	Y(2)=Y(2)+((Y(2)-Y)+H2*G1)*D(M+1))	F	50
	G1=V(M)-E	F	51
	D(M)=Y(2)/(1.-HV*G1)	F	52
COVERFLOW	F	53
	M1=M+1	F	54
	D1=D(M)	F	55

	DO 6 J=M1,M	F 56
6	P(J)=P(J)/DM	F 57
	V=V/DM	F 58
	V(2)=V(2)/DM	F 59
	V(3)=V(3)/DM	F 60
	G1=V(M+1)-F	F 61
	GO TO 5	F 62
CTEST FOR CROSSING PT.	F 63
	IF (ARSE(P(M))-ARSE(P(M+1))) 0,0,7	F 64
7	IF (M-2) 0,0,8	F 65
8	V=V(2)	F 66
	V(2)=V(2)	F 67
	M=M-1	F 68
	GO TO 5	F 69
C		F 70
9	DM=P(M)	F 71
	MSAVE=M	F 72
	V1N=V(2)/DM	F 73
	DO 10 J=M,M	F 74
10	P(J)=P(J)/DM	F 75
C		F 76
CSTART OUTWARD INTEGRATION	F 77
C		F 78
	P(1)=1.E-20	F 79
	V=0.	F 80
	G1=V-F	F 81
	V(2)=(1.-MV*G1)*P	F 82
	DO 13 I=2,M	F 83
11	V(3)=V(2)+((V(2)-V)+H2*G1*P(I-1))	F 84
	G1=V(I)-F	F 85
	P(I)=V(3)/(1.-MV*G1)	F 86
	I1=I-1	F 87
	DM=P(I1)	F 88
	DO 12 J=1,I1	F 89
12	P(J)=P(J)/DM	F 90
	V=V/DM	F 91
	V(2)=V(2)/DM	F 92
	V(3)=V(3)/DM	F 93
	G1=V(I1)-F	F 94
	GO TO 11	F 95
C		F 96
	V=V(2)	F 97
13	V(2)=V(2)	F 98
C		F 99
CFINISHED OUTWARD INTEGRATION	F 100
	DM=P(M)	F 101
	IF (DM) 14,17,14	F 102
14	VOU1T=Y/DM	F 103
	VM=V(3)/DM	F 104
	DO 15 J=1,M	F 105
15	P(J)=P(J)/DM	F 106
C		F 107
CCORRECTION	F 108
C		F 109
	DF=0.	F 110

	DO 14 J=1,N	F 111
16	DE=DE-D(J)**2	F 112
	F=(-YOUT-Y[N+2,*VM]/H2+(V(N)-F)	F 113
	DOLD=DE	F 114
17	F=9.999999E+20	F 115
	DE=-F	F 116
	DE=ARSE(.0001*F)	F 117
	GO TO 18	F 118
	DE=-F/DE	F 119
18	IF (N-1) 20,19,20	F 120
19	FPRIN=F*FACH	F 121
	DEPRIN=DE*FACH	F 122
	PRINT 45, 11,FPRIN,F,DE,DEPRIN,MSAVE	F 123
20	FOLD=F	F 124
	F=F+DE	F 125
	TEST=MAX1F(ARSE(DOLD)-ARSE(DE),TEST)	F 126
	IF (TEST) 22,21,21	F 127
21	IF (ARSE(F-FOLD)-ARSE(FPS)) 23,23,22	F 128
22	CONTINUE	F 129
	SCHR=1.	F 130
	GO TO 24	F 131
CCONVERGED-COUNT NODES	F 132
23	SCHR=0.	F 133
24	KV=0	F 134
	NL=N-2	F 135
	DO 34 J=2,NL	F 136
	IF (D(J)) 26,25,25	F 137
25	IF (D(J-1)) 27,34,34	F 138
26	IF (D(J-1)) 34,31,29	F 139
C	POS. NODE	F 140
27	IF (D(J+1)) 34,28,28	F 141
28	IF (D(J-2)) 32,34,34	F 142
C	NEG. NODE	F 143
29	IF (D(J+1)) 30,34,34	F 144
30	IF (D(J-2)) 34,33,33	F 145
C	FALSE NODE DUE TO UNDERFLOW	F 146
31	IF (D(J+1)) 32,34,34	F 147
32	IF (D(J-2)) 34,34,33	F 148
33	KV=KV+1	F 149
34	CONTINUE	F 150
CNORMALIZE	F 151
	SM=SORTE(-H*DE)	F 152
	DO 35 J=1,N	F 153
35	C(J)=P(J)/SM	F 154
CPRINT SOLUTION	F 155
	F=F*FACH	F 156
	IF (N-1) 38,36,38	F 157
36	IP51A=IP510*300	F 158
	IP51B=IP510*40	F 159
	IP51C=IP510*25	F 160
	IP51D=IP510*50	F 161
	DO 37 JF=1,N,IP51A	F 162
	PRINT 46, KV,N	F 163
	PRINT 46, KV,F	F 163
	J1=X*NOF(JF+IP51B,N)	F 164

	DO 37 J=JF, JL, IPSIC	F 165
	IL=XMINOF(J+IPSIC,N)	F 166
	PRINT 47, (I,S(I),I=J,IL,IPSIC)	F 167
37	CONTINUE	F 168
38	EO=F	F 169
	IF (NS-33) 40,39,40	F 170
39	PRINT 48, KV,F	F 171
40	CONTINUE	F 172
41	RETURN	F 173
C		F 174
42	DDRMJT (47015LOP- SOLUTION OF R1491L SCHR. EQUATION FOR V=13.5X.7H	F 175
42	FORMAT (47HISCHR- SOLUTION OF RADIAL SCHR. EQUATION FOR V=13.5X.7H	F 175
	1ETRIAL=1PE15.7.9H (1/CM)	F 176
43	FORMAT (70H1TER F F(F) DF(F)	F 177
	1 D(F))	F 178
44	FORMAT (50H DIFFERENCE EQUATION SOLUTION TECHNIQUE FAILS)	F 179
45	FORMAT (14014.2X,1P4E16.7.5X,29H THE CROSSING PT. OCCURS AT 14)	F 180
46	FORMAT (47HISCHR- SOLUTION OF RADIAL SCHR. EQUATION FOR V=13.7H	F 181
	1 F=1PE15.7/20H I S(1) S(20H I S(1))	F 182
47	FORMAT (6(15,1PE15.7))	F 183
48	FORMAT (50H SOLUTION OF RADIAL SCHR. EQUATION FOR V = 13.7H	F 184
	1 F = 1PE15.7)	F 185
	END	F 186-

```

SUBROUTINE SIMP (S,SS,M,H,RESULT)
C  INTEGRATION OF A PRODUCT S*SSBY SIMPSONS RULE.
  DIMENSION S(2000), SS(2000)
  SUM=0.0
  DO 1 J=2,M,2
1  SUM=SUM+2.0*S(J)*SS(J)+4.0*S(J-1)*SS(J-1)
  RESULT=SUM*H/3.0
  RETURN
END

```

```

G  1
G  2
G  3
G  4
G  5
G  6
G  7
G  8
G  9

```

APPENDIX III

TABLE OF R-CENTROIDS

Table 95

R-CENTROIDS FOR CN RED (1/2)

V	1	2	3	4	5	6	7	8	9
1	1.252-0	1.306-0	1.366-0	1.435-0	1.523-0	1.576-0	1.610-0	1.574-0	1.206-0
2	1.223-0	1.261-0	1.313-0	1.373-0	1.443-0	1.527-0	1.629-0	1.673-0	1.093-0
3	1.173-0	1.197-0	1.271-0	1.321-0	1.396-0	1.450-0	1.532-0	1.634-0	1.733-0
4	1.135-0	1.164-0	1.213-0	1.244-0	1.329-0	1.388-0	1.457-0	1.539-0	1.641-0
5	1.105-0	1.143-0	1.213-0	1.225-0	1.315-0	1.338-0	1.396-0	1.464-0	1.546-0
6	1.172-0	1.119-0	1.153-0	1.117-0	1.235-0	1.148-0	1.348-0	1.464-0	1.472-0
7	1.105-0	1.079-0	1.117-0	1.105-0	1.178-0	1.245-0	1.254-0	1.359-0	1.412-0
8	1.121-0	1.052-0	1.046-0	1.125-0	1.199-0	1.193-0	1.258-0	1.204-0	1.373-0
9	1.112-0	1.027-0	1.058-0	1.044-0	1.135-0	5.742-1	1.214-0	1.276-0	1.296-0
10	1.105-0	1.005-0	1.034-0	1.000-0	1.112-0	1.148-0	1.142-0	1.214-0	1.325-0
11	1.105-0	1.044-0	1.011-0	1.044-0	1.173-0	1.119-0	1.159-0	1.164-0	1.225-0
12	1.170-0	1.022-0	1.006-0	1.010-0	1.040-0	1.161-0	1.120-0	1.305-0	1.170-0
13	1.171-0	1.071-0	1.071-0	1.063-0	1.024-0	1.155-0	1.099-0	1.133-0	1.102-0
14	1.117-0	1.032-0	1.040-0	1.079-0	1.013-0	1.131-0	1.052-0	1.090-0	1.152-0
15	1.117-0	1.155-0	1.070-0	1.063-0	1.042-0	1.110-0	1.039-0	1.070-0	1.100-0
16	1.193-0	1.034-0	1.211-0	1.043-0	1.054-0	1.017-0	1.017-0	1.046-0	1.079-0
17	1.171-0	1.028-0	1.044-0	1.027-0	1.040-0	1.072-0	1.074-0	1.024-0	1.054-0
18	1.139-0	1.019-0	1.045-0	1.114-0	1.039-0	1.059-0	1.073-0	1.004-0	1.032-0
19	1.130-0	1.077-0	1.026-0	1.092-0	1.144-0	1.001-0	1.025-0	1.061-0	1.012-0

Table 95 (cont'd)

(CN 25) (1/2)

	10	11	12	13	14	15	16	17	18
1	1.000-0	1.237-0	1.743-0	1.910-0	1.372-0	1.395-0	1.231-0	1.322-0	1.327-0
2	1.021-0	1.090-0	1.339-0	1.234-0	1.316-0	1.315-0	1.471-0	1.364-0	1.523-0
3	1.044-0	1.033-0	1.133-0	1.240-0	1.242-0	1.223-0	1.326-0	1.515-0	1.332-0
4	1.069-0	1.031-0	1.117-0	1.134-0	1.433-0	1.044-0	1.142-0	1.549-0	1.314-0
5	1.097-0	1.073-0	2.023-0	1.022-0	1.270-0	1.429-0	1.251-0	2.106-0	3.175-0
6	1.124-0	1.055-0	1.741-0	1.935-0	2.741-0	1.325-0	3.220-0	1.309-0	1.214-0
7	1.147-0	1.052-0	1.603-0	1.737-0	1.903-0	1.742-0	1.541-0	3.702-0	6.690-0
8	1.171-0	1.044-0	1.509-0	1.670-0	1.810-0	2.056-0	1.800-0	1.000-0	1.363-0
9	1.196-0	1.029-0	1.446-0	1.577-0	1.679-0	1.814-0	2.976-0	2.051-0	1.694-0
10	1.221-0	1.005-0	1.403-0	1.504-0	1.543-0	1.588-0	1.823-0	2.139-0	1.955-0
11	1.246-0	1.010-0	1.344-0	1.449-0	1.513-0	1.593-0	1.636-0	1.829-0	2.055-0
12	1.271-0	1.032-0	1.329-0	1.331-0	1.451-0	1.521-0	1.632-0	1.704-0	1.840-0
13	1.296-0	1.054-0	1.254-0	1.341-0	1.360-0	1.474-0	1.531-0	1.610-0	1.713-0
14	1.321-0	1.076-0	1.230-0	1.274-0	1.356-0	1.477-0	1.491-0	1.540-0	1.619-0
15	1.346-0	1.098-0	1.211-0	1.397-0	1.247-0	1.375-0	1.390-0	1.514-0	1.570-0
16	1.371-0	1.051-0	1.104-0	1.224-0	1.149-0	1.299-0	1.410-0	1.402-0	1.563-0
17	1.396-0	1.040-0	1.140-0	1.179-0	1.239-0	1.223-0	1.311-0	1.569-0	1.412-0
18	1.421-0	1.039-0	1.199-0	1.135-0	1.190-0	1.262-0	1.247-0	1.325-0	1.227-0
19	1.446-0	1.071-0	1.112-0	9.951-1	1.130-0	1.212-0	1.326-0	1.263-0	1.343-0

Table 96

2-CENTROIDS FOR (24, 45) (3/2)

	1	2	3	4	5	6	7	8	9
1	1.233-0	1.304-0	1.361-0	1.433-0	1.509-0	1.579-0	1.657-0	1.729-0	1.805-0
2	1.221-0	1.291-0	1.343-0	1.395-0	1.447-0	1.499-0	1.551-0	1.603-0	1.655-0
3	1.173-0	1.149-0	1.271-0	1.321-0	1.373-0	1.425-0	1.477-0	1.529-0	1.581-0
4	1.135-0	1.143-0	1.214-0	1.245-0	1.329-0	1.389-0	1.449-0	1.509-0	1.569-0
5	1.102-0	1.143-0	1.205-0	1.275-0	1.315-0	1.375-0	1.435-0	1.495-0	1.555-0
6	1.053-0	1.108-0	1.151-0	1.193-0	1.235-0	1.277-0	1.319-0	1.361-0	1.403-0
7	1.014-0	1.077-0	1.116-0	1.152-0	1.188-0	1.224-0	1.260-0	1.296-0	1.332-0
8	0.9821-1	1.047-0	1.094-0	1.124-0	1.150-0	1.176-0	1.202-0	1.228-0	1.254-0
9	0.9492-1	1.021-0	1.155-0	1.191-0	1.132-0	1.163-0	1.194-0	1.225-0	1.256-0
10	0.9244-1	0.984-1	1.028-0	1.052-0	1.133-0	1.143-0	1.174-0	1.205-0	1.236-0
11	0.8973-1	0.775-1	1.003-0	1.035-0	1.070-0	1.117-0	1.150-0	1.184-0	1.225-0
12	0.8710-1	0.545-1	0.819-1	1.010-0	1.043-0	1.077-0	1.116-0	1.197-0	1.177-0
13	0.8440-1	0.257-1	0.617-1	0.871-1	1.017-0	1.053-0	1.035-0	1.126-0	1.061-0
14	0.8174-1	0.913-1	0.391-1	0.655-1	0.937-1	1.025-0	1.037-0	1.093-0	1.130-0
15	0.7904-1	0.594-1	0.102-1	0.404-1	0.719-1	1.011-0	1.032-0	1.065-0	1.101-0
16	0.7634-1	0.444-1	0.749-1	0.233-1	0.510-1	0.793-1	1.019-0	1.139-0	1.073-0
17	0.7364-1	0.517-1	0.447-1	0.934-1	0.310-1	0.572-1	0.833-1	1.015-0	1.047-0
18	0.7094-1	0.656-1	0.219-1	0.554-1	0.053-1	0.359-1	0.639-1	0.926-1	1.023-0
19	0.6824-1	0.591-1	0.233-1	0.111-1	0.742-1	0.154-1	0.434-1	0.711-1	1.000-0

Table 96 (cont'd)

(CN 2E) (3/21)

	10	11	12	13	14	15	16	17	18
1	1.673-0	1.317-0	1.401-0	1.324-0	1.367-0	1.290-0	1.034-0	1.314-0	1.240-0
2	1.241-0	1.121-0	1.337-0	1.272-0	1.553-0	1.335-0	1.531-0	1.339-0	1.137-0
3	2.941-1	1.255-0	1.195-0	1.543-0	1.271-0	1.050-0	1.413-0	1.267-0	1.635-0
4	1.640-0	3.996-0	1.240-0	1.443-0	2.477-0	1.262-0	1.171-0	1.544-0	1.306-0
5	1.602-0	1.737-0	2.517-0	1.224-0	1.142-0	5.842-0	1.259-0	1.165-0	4.842-1
6	1.500-0	1.609-0	1.754-0	2.322-0	1.141-0	1.267-0	1.220-0	1.261-0	1.193-0
7	1.441-0	1.507-0	1.670-0	1.745-0	2.174-0	1.165-0	1.140-0	0.729-1	1.216-0
8	1.421-0	1.490-0	1.575-0	1.644-0	1.415-0	2.255-0	1.161-0	1.234-0	2.240-0
9	1.344-0	1.431-0	1.494-0	1.593-0	1.533-0	1.924-0	2.242-0	4.331-1	1.305-0
10	1.270-0	1.440-0	1.440-0	1.507-0	1.532-0	1.762-0	1.036-0	2.181-0	2.200-0
11	2.121-0	1.317-0	9.939-0	1.451-0	1.516-0	1.600-0	1.711-0	1.847-0	2.174-0
12	1.230-0	1.213-0	1.320-0	1.301-0	1.452-0	1.525-0	1.039-0	1.719-0	1.860-0
13	1.144-0	1.250-0	1.252-0	1.340-0	1.349-0	1.475-0	1.534-0	1.010-0	1.729-0
14	1.130-0	1.199-0	1.270-0	1.270-0	1.353-0	1.371-0	1.490-0	1.544-0	1.627-0
15	1.161-0	1.154-0	1.210-0	1.312-0	1.243-0	1.369-0	1.346-0	1.508-0	1.554-0
16	1.111-0	1.421-0	1.107-0	1.221-0	4.434-0	1.296-0	1.392-0	1.399-0	1.536-0
17	1.041-0	1.123-0	1.113-0	1.179-0	1.244-0	1.199-0	1.308-0	1.436-0	1.410-0
18	1.000-0	1.090-0	1.140-0	1.133-0	1.144-0	1.250-0	1.234-0	1.321-0	1.700-0
19	1.031-0	1.003-0	1.099-0	1.195-0	1.144-0	1.199-0	1.275-0	1.255-0	1.335-0

Table 97

X-CENTROIDS FOR (CN VIOLET)

<i>N</i>	<i>N</i>	1	2	3	4	5	6	7	8	9
1	1.110-0	1.152-0	9.735-1	9.270-1	9.952-1	9.139-1	3.554-0	1.227-0	1.167-0	3.339-0
2	1.214-0	1.173-0	1.057-0	9.463-1	9.157-1	9.541-1	7.876-1	9.137-1	1.316-0	1.144-0
3	1.413-0	1.212-0	1.147-0	9.159-0	9.942-1	9.158-1	9.489-1	7.489-1	3.056-1	1.650-0
4	2.423-0	1.353-0	1.353-0	1.139-0	1.054-0	9.954-1	9.149-1	8.452-1	7.515-1	5.241-1
5	1.314-0	3.746-1	1.552-0	1.315-0	1.212-0	1.154-0	1.071-0	9.150-1	9.553-1	7.463-1
6	1.224-0	1.511-0	8.653-1	1.590-0	1.328-0	1.225-0	1.546-0	1.009-0	9.111-1	9.554-1
7	1.115-0	1.274-0	1.533-0	1.055-0	1.674-0	1.343-0	1.242-0	1.029-0	1.119-0	9.034-1
8	1.359-0	1.144-0	1.377-0	1.654-0	1.173-0	1.445-0	1.260-0	1.253-0	9.973-1	1.032-0
9	1.145-0	3.543-0	1.249-0	1.462-0	1.773-0	1.253-0	2.559-0	1.340-0	1.276-0	9.456-1
10	1.777-0	1.172-0	1.409-0	1.339-0	1.141-0	2.125-0	1.230-0	1.357-0	1.404-0	1.291-0
11	1.444-0	1.225-0	1.174-0	9.913-1	1.525-0	1.383-0	7.580-0	1.331-0	7.980-1	1.434-0
12	1.246-0	1.137-0	1.131-0	1.142-0	2.443-0	1.559-0	1.447-0	6.374-1	1.458-0	1.041-0
13	1.123-0	1.334-0	9.949-1	1.175-0	1.241-0	1.190-0	1.084-0	1.625-0	1.062-0	1.554-0
14	1.300-0	1.177-0	1.316-0	1.145-0	9.940-1	1.555-0	1.255-0	1.210-0	1.910-0	1.222-0
15	1.777-0	1.132-0	1.130-0	1.265-0	1.237-0	1.299-0	1.341-0	1.478-0	1.413-0	5.224-0
16	1.444-0	1.123-0	1.079-0	1.193-0	1.457-0	1.511-0	1.447-0	1.234-0	1.404-0	1.546-0
17	1.143-0	2.417-0	1.077-0	1.126-0	1.112-0	2.117-0	1.216-0	1.979-0	1.386-0	1.097-0
18	1.213-0	1.353-0	1.031-0	9.774-1	1.244-0	1.541-0	1.543-0	1.336-0	9.549-1	1.549-0
19	1.213-0	1.241-0	2.002-0	5.755-1	1.113-0	3.453-1	1.259-0	1.016-0	1.495-0	1.354-0

Table 97 (cont'd)

(CN VIOLET)

ν	ν/cm^{-1}	11	12	13	14	15	16	17	18
1	1.237-0	1.344-0	8.345-1	9.412-1	1.215-0	9.026-1	1.357-0	1.100-0	1.170-0
2	1.691-1	1.231-0	1.129-0	1.323-0	1.341-0	1.141-0	1.040-0	9.009-1	9.250-1
3	1.214-0	1.325-0	1.239-0	1.164-0	1.146-0	1.142-0	1.128-0	1.131-0	1.030-0
4	3.214-0	1.311-0	1.030-0	1.126-0	1.434-0	3.336-0	9.822-1	1.054-0	1.032-0
5	5.555-1	7.773-1	1.325-0	1.134-0	3.159-1	1.758-0	6.835-1	1.056-0	1.033-0
6	7.910-1	4.745-1	7.552-1	1.305-0	1.129-0	1.053-0	7.441-1	9.309-1	6.179-1
7	4.522-1	7.530-1	4.596-1	4.145-0	1.249-0	1.074-0	1.045-0	9.986-1	3.314-1
8	4.945-1	8.468-1	7.427-1	4.374-1	3.813-0	1.296-0	1.074-0	9.969-1	9.734-1
9	1.049-0	4.745-1	6.515-1	7.211-1	4.413-1	3.533-0	1.314-0	1.090-0	9.494-1
10	3.614-1	1.074-0	8.405-1	9.610-1	3.919-1	4.983-1	3.838-0	1.332-0	1.119-0
11	1.314-0	5.933-1	1.119-0	7.793-1	4.853-1	6.261-1	5.560-1	5.328-0	1.400-0
12	1.474-0	1.316-0	3.371-1	1.151-0	6.512-1	9.402-1	4.935-1	7.003-1	9.706-1
13	1.204-0	1.540-0	1.325-0	1.273-0	1.213-0	3.035-1	1.038-0	9.624-1	8.112-1
14	1.754-0	1.230-0	1.018-0	1.371-0	1.244-0	1.260-0	1.246-0	1.150-0	1.073-0
15	1.325-0	2.913-0	1.335-0	2.771-0	1.330-0	3.508-0	1.319-0	5.062-0	1.257-0
16	5.276-1	1.418-0	5.194-1	1.347-0	4.657-1	1.320-0	2.520-0	1.364-0	2.640-0
17	1.742-0	1.045-0	1.516-0	1.072-0	1.442-0	1.179-0	1.238-0	2.398-0	1.400-0
18	1.368-0	2.550-0	1.246-0	1.725-0	1.233-0	1.524-0	1.252-0	1.247-0	2.377-0
19	4.115-1	1.513-0	2.549-1	1.354-0	3.453-0	1.319-0	1.745-0	1.298-0	1.131-0

Table 98

O-CENTRATIONS FOR (C) + (M +)

	1	2	3	4	5	6	7	8	9	10	11	12
1	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
2	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
3	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
4	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
5	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
6	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
7	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
8	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
9	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
10	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
11	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
12	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
13	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
14	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
15	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
16	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
17	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
18	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
19	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0
20	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0	1.000-0

Table 98 (cont'd)

(CO 474 +)

	13	14	15	15	17	18	19	20	21	22	23	24
1	1.372-0	1.531-0	1.240-0	0.955-1	1.325-0	1.120-0	9.412-1	1.447-0	1.242-0	2.311-1	0.809-1	1.176-0
2	1.540-0	1.538-0	1.705-0	1.264-0	1.115-0	1.330-0	1.027-0	1.177-1	1.120-0	1.126-0	1.235-0	1.224-0
3	1.525-0	1.546-0	1.545-0	3.363-0	1.129-0	1.441-0	1.343-0	1.259-0	1.410-0	1.252-0	5.916-0	1.636-0
4	1.511-0	1.538-0	1.503-0	1.702-0	1.443-0	1.510-0	1.523-0	1.255-0	1.403-0	1.703-0	1.335-0	1.196-0
5	1.447-0	1.514-0	1.533-0	1.590-0	1.639-0	1.649-0	1.549-0	1.732-0	1.353-0	1.590-0	1.444-0	1.437-0
6	1.466-0	1.436-0	1.528-0	1.501-0	1.593-0	1.622-0	1.642-0	1.636-0	2.160-0	1.322-0	1.431-0	1.491-0
7	1.445-0	1.475-0	1.535-0	1.536-0	1.567-0	1.539-0	1.620-0	1.639-0	1.739-0	2.006-0	1.997-0	1.522-0
8	1.428-0	1.455-0	1.444-0	1.513-0	1.544-0	1.575-0	1.606-0	1.643-0	1.677-0	1.717-0	1.702-0	1.736-0
9	1.402-0	1.429-0	1.405-0	1.443-0	1.522-0	1.533-0	1.546-0	1.616-0	1.649-0	1.683-0	1.711-0	1.754-0
10	1.388-0	1.413-0	1.441-0	1.445-0	1.533-0	1.532-0	1.562-0	1.593-0	1.624-0	1.656-0	1.690-0	1.725-0
11	1.364-0	1.398-0	1.424-0	1.452-0	1.477-0	1.517-0	1.542-0	1.571-0	1.602-0	1.633-0	1.665-0	1.700-0
12	1.335-0	1.376-0	1.413-0	1.433-0	1.462-0	1.499-0	1.475-0	1.553-0	1.591-0	1.611-0	1.643-0	1.675-0
13	1.332-0	1.356-0	1.390-0	1.415-0	1.439-0	1.475-0	1.511-0	1.526-0	1.569-0	1.592-0	1.622-0	1.653-0
14	1.313-0	1.351-0	1.369-0	1.391-0	1.426-0	1.453-0	1.519-0	1.513-0	1.539-0	1.555-0	1.615-0	1.633-0
15	1.287-0	1.326-0	1.347-0	1.342-0	1.437-0	1.443-0	1.465-0	1.490-0	1.527-0	1.550-0	1.575-0	1.636-0
16	1.287-0	1.340-0	1.342-0	1.364-0	1.399-0	1.420-0	1.441-0	1.477-0	1.503-0	1.475-0	1.503-0	1.597-0
17	1.271-0	1.233-0	1.323-0	1.333-0	1.377-0	1.401-0	1.434-0	1.457-0	1.499-0	1.516-0	1.539-0	1.591-0
18	1.256-0	1.246-0	1.316-0	1.333-0	1.365-0	1.392-0	1.416-0	1.453-0	1.471-0	1.494-0	1.530-0	1.553-0
19	1.241-0	1.271-0	1.103-0	1.322-0	1.200-0	1.374-0	1.395-0	1.430-0	1.452-0	1.487-0	1.510-0	1.625-0
20	1.232-0	1.277-0	1.237-0	1.337-0	1.340-0	1.350-0	1.390-0	1.415-0	1.449-0	1.469-0	1.439-0	1.524-0
21	1.223-0	1.244-0	5.233-0	1.231-0	1.579-0	1.342-0	2.682-0	1.339-0	1.446-0	6.970-0	1.300-0	5.446-0

Table 99

Q-CENTROIDS FOR (M(2) 1ST. 0)

V	1	2	3	4	5	6
1	1.210-0	1.113-0	1.152-0	1.125-0	1.103-0	1.077-0
2	1.317-0	1.227-0	1.192-0	1.151-0	1.133-0	1.119-0
3	1.313-0	1.257-0	1.249-0	1.213-0	1.171-0	1.142-0
4	1.357-0	1.323-0	1.271-0	1.139-0	1.219-0	1.141-0
5	1.412-0	1.357-0	1.357-0	1.243-0	1.236-0	1.271-0
6	1.547-0	1.421-0	1.373-0	1.247-0	1.296-0	1.249-0
7	1.657-0	1.496-0	1.431-0	1.310-0	1.322-0	1.315-0
8	1.774-0	1.564-0	1.495-0	1.441-0	1.407-0	1.377-0
9	2.033-0	1.656-0	1.574-0	1.515-0	1.452-0	1.439-0
10	1.145-0	1.749-0	1.675-0	1.544-0	1.515-0	1.453-0
11	1.195-0	2.042-0	1.913-0	1.616-0	1.593-0	1.525-0
12	1.018-0	1.369-0	2.063-0	1.931-0	1.696-0	1.637-0
13	1.270-0	1.245-0	2.059-0	2.031-0	1.840-0	1.717-0
14	1.205-0	1.506-0	1.335-0	3.034-0	2.099-0	1.853-0
15	3.517-1	1.240-0	1.722-0	1.523-0	5.097-0	2.144-0
16	1.355-0	4.213-1	1.316-0	3.450-0	1.397-0	3.349-0
17	1.316-0	5.431-1	1.219-0	1.170-0	1.064-0	1.427-0
18	1.331-0	1.331-0	2.195-0	1.232-0	9.941-1	1.031-0

(N(2) 1ST. 4)

Table 99 (cont'd)

V	VV	7	4	9	10	11	12	13
1	1.0350-0	1.030-0	1.019-0	9.990-1	9.927-1	9.680-1	9.563-1	
2	1.0345-0	1.064-0	1.044-0	1.026-0	1.019-0	9.920-1	9.775-1	
3	1.0330-0	1.093-0	1.072-0	1.053-0	1.035-0	1.019-0	1.002-0	
4	1.0315-0	1.126-0	1.102-0	1.081-0	1.061-0	1.043-0	1.026-0	
5	1.0300-0	1.162-0	1.135-0	1.111-0	1.090-0	1.073-0	1.052-0	
6	1.0285-0	1.204-0	1.173-0	1.145-0	1.121-0	1.099-0	1.079-0	
7	1.0270-0	1.244-0	1.208-0	1.174-0	1.150-0	1.131-0	1.109-0	
8	1.0255-0	1.284-0	1.233-0	1.195-0	1.173-0	1.170-0	1.142-0	
9	1.0240-0	1.323-0	1.259-0	1.215-0	1.206-0	1.111-0	1.141-0	
10	1.0225-0	1.363-0	1.298-0	1.254-0	1.259-0	1.221-0	1.193-0	
11	1.0210-0	1.402-0	1.337-0	1.317-0	1.317-0	1.274-0	1.234-0	
12	1.0195-0	1.443-0	1.373-0	1.395-0	1.395-0	1.251-0	1.295-0	
13	1.0180-0	1.484-0	1.407-0	1.414-0	1.425-0	1.347-0	1.230-0	
14	1.0165-0	1.525-0	1.448-0	1.430-0	1.430-0	1.320-0	1.352-0	
15	1.0150-0	1.566-0	1.489-0	1.471-0	1.472-0	1.444-0	1.257-0	
16	1.0135-0	1.607-0	1.529-0	1.503-0	1.503-0	1.749-0	1.459-0	
17	1.0120-0	1.648-0	1.569-0	1.553-0	1.553-0	1.598-0	1.236-0	
18	1.0105-0	1.689-0	1.609-0	1.597-0	1.597-0	1.572-0	1.615-0	

Table 100

R-CENTROIDS FOR (M(2) 2ND. +)

ν	ν	1	2	3	4	5	7	8
1	1.146-	1.147-	1.114-	1.033-0	1.055-0	1.014-0	9.799-1	9.561-1
2	1.210-	1.210-	1.155-0	1.121-0	1.062-0	1.036-0	1.011-0	9.671-1
3	1.233-	1.233-	1.154-0	1.155-0	1.129-0	1.099-0	1.043-0	1.014-0
4	1.249-	1.249-	1.205-0	1.143-0	1.114-0	1.137-0	1.076-0	1.049-0
5	1.355-	1.354-0	1.313-0	1.231-0	1.134-0	1.150-0	1.111-0	1.042-0

ν	ν	10	11	12	13	14	15	16	17
1	3.014-	3.009-1	8.425-1	9.614-1	8.455-1	8.392-1	8.341-1	8.394-1	8.353-1
2	3.041-	3.013-1	9.143-1	9.951-1	9.729-1	8.545-1	8.420-1	8.329-1	8.143-1
3	3.052-	3.016-1	9.435-1	9.291-1	9.157-1	8.847-1	8.622-1	8.405-1	8.145-1
4	3.059-	1.011-0	9.733-1	9.570-1	9.358-1	9.153-1	8.945-1	8.713-1	8.423-1
5	3.059-	1.030-0	1.057-0	9.854-1	9.639-1	9.423-1	9.210-1	9.001-1	8.742-1

Table 101

R-CENTROIDS FOR (12 3-M 1)

	VV	1	2	3	4	5	6	7	8	9	10
1	1.200-0	1.224-0	1.242-0	1.242-0	1.276-0	1.292-0	1.309-0	1.325-0	1.341-0	1.357-0	1.373-0
2	1.200-0	1.218-0	1.236-0	1.236-0	1.270-0	1.287-0	1.303-0	1.319-0	1.336-0	1.352-0	1.367-0
3	1.200-0	1.213-0	1.230-0	1.230-0	1.265-0	1.281-0	1.298-0	1.314-0	1.330-0	1.346-0	1.361-0
4	1.200-0	1.207-0	1.225-0	1.225-0	1.259-0	1.276-0	1.292-0	1.308-0	1.324-0	1.339-0	1.355-0
5	1.200-0	1.201-0	1.219-0	1.219-0	1.254-0	1.270-0	1.287-0	1.303-0	1.317-0	1.336-0	1.351-0
6	1.176-0	1.196-0	1.214-0	1.214-0	1.249-0	1.265-0	1.281-0	1.297-0	1.314-0	1.329-0	1.345-0
7	1.176-0	1.190-0	1.209-0	1.209-0	1.243-0	1.260-0	1.276-0	1.292-0	1.308-0	1.323-0	1.338-0
8	1.176-0	1.184-0	1.203-0	1.203-0	1.238-0	1.255-0	1.271-0	1.287-0	1.302-0	1.317-0	1.335-0
9	1.158-0	1.179-0	1.198-0	1.198-0	1.234-0	1.248-0	1.265-0	1.281-0	1.297-0	1.314-0	1.329-0
10	1.151-0	1.173-0	1.193-0	1.193-0	1.223-0	1.243-0	1.260-0	1.276-0	1.292-0	1.308-0	1.323-0
11	1.145-0	1.168-0	1.188-0	1.188-0	1.221-0	1.239-0	1.255-0	1.270-0	1.287-0	1.302-0	1.316-0
12	1.132-0	1.158-0	1.183-0	1.183-0	1.216-0	1.233-0	1.254-0	1.266-0	1.282-0	1.297-0	1.313-0
13	1.125-0	1.154-0	1.181-0	1.181-0	1.211-0	1.229-0	1.244-0	1.261-0	1.277-0	1.293-0	1.308-0
14	1.118-0	1.151-0	1.180-0	1.180-0	1.207-0	1.212-0	1.239-0	1.256-0	1.270-0	1.287-0	1.302-0
15	1.111-0	1.156-0	1.187-0	1.187-0	1.226-0	1.213-0	1.230-0	1.243-0	1.262-0	1.270-0	1.294-0
16	1.104-0	1.325-0	1.154-0	1.154-0	1.190-0	1.219-0	1.226-0	1.240-0	1.257-0	1.263-0	1.289-0
17	1.096-0	1.080-0	1.150-0	1.150-0	1.186-0	1.205-0	1.220-0	1.236-0	1.254-0	1.267-0	1.284-0
18	1.090-0	1.098-0	1.149-0	1.149-0	1.183-0	1.213-0	1.216-0	1.231-0	1.243-0	1.263-0	1.280-0
19	1.079-0	1.096-0	1.150-0	1.150-0	1.180-0	1.212-0	1.212-0	1.226-0	1.242-0	1.259-0	1.283-0
20	1.068-0	1.091-0	1.182-0	1.182-0	1.179-0	1.217-0	1.208-0	1.226-0	1.237-0	1.253-0	1.267-0

Table 191 (cont'd)

(112) 3-4 1)

	11	12	13	14	15	16	17	18	19	20	21
1	1.531-0	1.410-0	1.422-0	1.439-0	1.455-0	1.472-0	1.490-0	1.507-0	1.525-0	1.543-0	1.562-0
2	1.535-0	1.413-0	1.415-0	1.430-0	1.459-0	1.489-0	1.504-0	1.531-0	1.510-0	1.536-0	1.555-0
3	1.537-0	1.412-0	1.411-0	1.427-0	1.457-0	1.475-0	1.493-0	1.499-0	1.520-0	1.532-0	1.549-0
4	1.537-0	1.414-0	1.414-0	1.419-0	1.434-0	1.459-0	1.471-0	1.497-0	1.533-0	1.519-0	1.530-0
5	1.536-0	1.412-0	1.405-0	1.414-0	1.431-0	1.447-0	1.462-0	1.476-0	1.505-0	1.516-0	1.532-0
6	1.536-0	1.419-0	1.433-0	1.444-0	1.463-0	1.487-0	1.511-0	1.474-0	1.489-0	1.514-0	1.534-0
7	1.536-0	1.411-0	1.436-0	1.441-0	1.459-0	1.485-0	1.459-0	1.465-0	1.465-0	1.502-0	1.517-0
8	1.534-0	1.415-0	1.437-0	1.439-0	1.413-0	1.427-0	1.443-0	1.454-0	1.477-0	1.492-0	1.502-0
9	1.534-0	1.415-0	1.437-0	1.431-0	1.445-0	1.462-0	1.439-0	1.454-0	1.467-0	1.497-0	1.504-0
10	1.534-0	1.415-0	1.437-0	1.433-0	1.447-0	1.467-0	1.431-0	1.442-0	1.467-0	1.480-0	1.493-0
11	1.534-0	1.434-0	1.403-0	1.433-0	1.435-0	1.413-0	1.433-0	1.443-0	1.457-0	1.469-0	1.494-0
12	1.532-0	1.432-0	1.462-0	1.434-0	1.444-0	1.445-0	1.421-0	1.435-0	1.443-0	1.469-0	1.482-0
13	1.474-0	1.534-0	1.454-0	1.436-0	1.413-0	1.410-0	1.414-0	1.413-0	1.447-0	1.460-0	1.469-0
14	1.313-0	1.328-0	1.340-0	1.359-0	1.373-0	1.383-0	1.394-0	1.426-0	1.439-0	1.442-0	1.472-0
15	1.313-0	1.328-0	1.340-0	1.359-0	1.373-0	1.380-0	1.405-0	1.418-0	1.420-0	1.451-0	1.463-0
16	1.314-0	1.322-0	1.339-0	1.353-0	1.364-0	1.395-0	1.398-0	1.437-0	1.432-0	1.443-0	1.433-0
17	1.292-0	1.321-0	1.333-0	1.347-0	1.365-0	1.378-0	1.388-0	1.409-0	1.423-0	1.426-0	1.455-0
18	1.292-0	1.314-0	1.328-0	1.346-0	1.359-0	1.371-0	1.392-0	1.432-0	1.413-0	1.435-0	1.447-0
19	1.295-0	1.319-0	1.315-0	1.339-0	1.353-0	1.374-0	1.394-0	1.394-0	1.415-0	1.427-0	1.433-0
20	1.291-0	1.314-0	1.322-0	1.333-0	1.344-0	1.364-0	1.378-0	1.411-0	1.407-0	1.413-0	1.439-0
21	1.295-0	1.311-0	1.315-0	1.324-0	1.344-0	1.357-0	1.378-0	1.399-0	1.399-0	1.419-0	1.430-0

Table 102

R-CENTROIDS FOR (V2 3-M 2)

V	1	2	3	4	5	7	9	10
1	1.114-0	1.212-0	1.212-0	1.237-0	1.274-0	1.317-0	1.336-0	1.373-0
2	1.114-0	1.216-0	1.206-0	1.252-0	1.274-0	1.311-0	1.331-0	1.368-0
3	1.117-0	1.210-0	1.200-0	1.234-0	1.255-0	1.306-0	1.325-0	1.370-0
4	1.112-0	1.205-0	1.205-0	1.237-0	1.250-0	1.317-0	1.318-0	1.355-0
5	1.116-0	1.170-0	1.170-0	1.232-0	1.259-0	1.292-0	1.312-0	1.346-0
6	1.114-0	1.107-0	1.107-0	1.243-0	1.242-0	1.296-0	1.309-0	1.342-0
7	1.113-0	1.159-0	1.159-0	1.244-0	1.237-0	1.274-0	1.297-0	1.335-0
8	1.113-0	1.151-0	1.151-0	1.244-0	1.233-0	1.271-0	1.291-0	1.327-0
9	1.113-0	1.144-0	1.144-0	1.243-0	1.241-0	1.265-0	1.291-0	1.320-0
10	1.112-0	1.137-0	1.137-0	1.242-0	1.236-0	1.271-0	1.275-0	1.313-0
11	1.111-0	1.110-0	1.110-0	1.121-0	1.203-0	1.243-0	1.270-0	1.317-0
12	1.109-0	1.103-0	1.103-0	1.155-0	1.139-0	1.240-0	1.260-0	1.311-0
13	1.108-0	1.094-0	1.094-0	1.151-0	1.211-0	1.235-0	2.341-1	1.296-0
14	1.107-0	1.084-0	1.084-0	1.144-0	1.342-0	1.233-0	1.243-0	1.310-0
15	1.106-0	1.074-0	1.074-0	1.136-0	1.140-0	7.167-1	1.240-0	1.276-0
16	1.105-0	1.064-0	1.064-0	1.127-0	1.145-0	1.235-0	1.236-0	1.273-0
17	1.104-0	1.055-0	1.055-0	1.116-0	1.142-0	1.233-0	1.235-0	1.268-0
18	1.103-0	1.046-0	1.046-0	1.100-0	1.135-0	1.230-0	1.247-0	1.263-0
19	1.102-0	1.037-0	1.037-0	1.083-0	1.128-0	1.137-0	1.143-0	1.261-0
20	1.101-0	1.029-0	1.029-0	1.114-0	1.120-0	1.136-0	1.199-0	1.250-0
21	1.100-0	1.021-0	1.021-0	1.113-0	1.111-0	1.231-0	1.194-0	1.240-0
22	1.099-0	1.014-0	1.014-0	1.094-0	1.110-0	1.239-0	1.196-0	1.245-0
23	1.098-0	1.009-0	1.009-0	1.093-0	1.093-0	1.001-1	1.193-0	1.242-0
24	1.097-0	1.002-0	1.002-0	1.079-0	1.097-0	1.119-0	1.190-0	1.240-0
25	1.096-0	1.000-0	1.000-0	1.073-0	1.114-0	1.128-0	1.199-0	1.240-0

Table 102 (cont'd)

(N(2) 3-4 2)

	11	12	13	14	15	16	17	18	19	20	21
1	1.342-0	1.411-0	1.424-0	1.446-0	1.455-0	1.444-0	1.503-0	1.523-0	1.543-0	1.564-0	1.545-0
2	1.340-0	1.414-0	1.422-0	1.440-0	1.459-0	1.477-0	1.496-0	1.516-0	1.536-0	1.556-0	1.577-0
3	1.341-0	1.413-0	1.416-0	1.434-0	1.453-0	1.471-0	1.490-0	1.509-0	1.529-0	1.549-0	1.570-0
4	1.343-0	1.415-0	1.412-0	1.429-0	1.447-0	1.465-0	1.483-0	1.502-0	1.521-0	1.541-0	1.562-0
5	1.347-0	1.419-0	1.413-0	1.420-0	1.438-0	1.454-0	1.477-0	1.495-0	1.514-0	1.533-0	1.554-0
6	1.359-0	1.437-0	1.439-0	1.444-0	1.431-0	1.449-0	1.465-0	2.000-0	1.508-0	1.526-0	1.546-0
7	1.355-0	1.431-0	1.434-0	1.445-0	1.439-0	1.444-0	1.460-0	1.477-0	1.494-0	1.465-0	1.542-0
8	1.346-0	1.433-0	1.436-0	1.440-0	1.417-0	1.433-0	1.446-0	1.473-0	1.489-0	1.516-0	1.521-0
9	1.340-0	1.434-0	1.434-0	1.441-0	1.447-0	1.430-0	1.445-0	1.451-0	1.475-0	1.515-0	1.519-0
10	1.330-0	1.435-0	1.437-0	1.434-0	1.442-0	1.419-0	1.433-0	1.459-0	1.473-0	1.449-0	1.498-0
11	1.324-0	1.433-0	1.431-0	1.430-0	1.394-0	1.346-0	1.431-0	1.447-0	1.460-0	1.449-0	1.531-0
12	1.317-0	1.434-0	1.434-0	1.371-0	1.394-0	1.415-0	1.422-0	1.429-0	1.460-0	1.474-0	1.447-0
13	1.316-0	1.429-0	1.437-0	1.364-0	1.343-0	1.347-0	1.434-0	1.434-0	1.450-0	1.452-0	1.447-0
14	1.317-0	1.422-0	1.434-0	1.350-0	1.376-0	1.419-0	1.416-0	1.425-0	1.434-0	1.463-0	1.476-0
15	1.312-0	1.414-0	1.434-0	1.351-0	1.374-0	1.344-0	1.462-0	1.293-0	1.434-0	1.454-0	1.375-0
16	1.240-0	1.314-0	1.329-0	1.344-0	1.362-0	1.341-0	1.385-0	1.415-0	1.429-0	1.427-0	1.467-0
17	1.259-0	1.344-0	1.323-0	1.343-0	1.356-0	1.376-0	1.394-0	1.400-0	1.414-0	1.442-0	1.458-0
18	1.274-0	1.363-0	1.318-0	1.356-0	1.350-0	1.366-0	1.387-0	1.400-0	1.423-0	1.434-0	1.449-0
19	1.273-0	1.340-0	1.313-0	1.331-0	1.314-0	1.352-0	1.382-0	1.414-0	1.415-0	1.425-0	1.448-0
20	1.269-0	1.344-0	1.319-0	1.327-0	1.347-0	1.357-0	1.378-0	1.394-0	1.404-0	1.443-0	1.441-0
21	1.265-0	1.270-0	1.344-0	1.325-0	1.347-0	1.331-0	1.358-0	1.398-0	1.401-0	1.424-0	1.434-0
22	1.261-0	1.275-0	1.341-0	1.310-0	1.335-0	1.342-0	1.365-0	1.393-0	1.412-0	1.417-0	1.424-0
23	1.257-0	1.273-0	1.299-0	1.310-0	1.332-0	1.348-0	1.361-0	1.379-0	1.396-0	1.413-0	1.459-0
24	1.250-0	1.270-0	1.314-0	1.317-0	1.329-0	1.346-0	1.356-0	1.376-0	1.391-0	1.417-0	1.427-0
25	1.251-0	1.260-0	1.205-0	1.344-0	1.332-0	1.341-0	1.351-0	1.370-0	1.346-0	1.425-0	1.422-0

Table 103

R-CENTROIDS FOR (42° MEINEL)

V	0	1	2	3	4	5	6	7	8	9	10	11	12
1	1.157-1	1.131-1	1.231-1	1.275-0	1.332-0	1.430-0	1.402-0	1.454-1	2.042-0	1.240-1	7.733-1	1.274-0	1.141-1
2	1.160-1	1.131-1	1.231-1	1.238-0	1.293-0	1.330-1	1.433-0	1.403-0	1.513-0	2.931-1	1.253-0	1.334-0	1.405-0
3	1.164-1	1.133-1	1.159-0	1.221-1	1.247-0	1.291-1	1.344-0	1.413-0	1.494-0	1.574-1	2.974-1	1.274-0	1.371-1
4	1.175-0	1.140-0	1.231-0	1.109-0	1.125-0	1.257-1	1.239-0	1.352-0	1.419-0	1.512-1	1.663-0	1.314-0	1.314-0
5	1.182-1	1.141-1	1.115-1	1.129-1	1.130-1	1.136-1	1.271-1	1.300-0	1.359-0	1.420-1	1.526-0	1.750-1	1.304-1
6	1.132-1	1.129-1	1.044-1	1.134-1	1.141-0	1.194-1	1.214-0	1.494-0	1.315-0	1.307-1	1.437-0	1.033-0	1.743-0
7	1.013-0	1.131-1	1.055-1	1.095-0	1.140-0	1.151-1	1.237-1	1.221-0	1.544-0	1.326-1	1.376-0	1.445-0	1.553-0
8	1.095-1	1.141-1	1.143-1	1.071-1	1.100-0	1.112-1	1.161-1	1.125-0	1.230-0	1.242-1	1.338-0	1.305-0	1.455-0
9	1.080-1	1.144-1	1.123-1	1.049-0	1.077-0	1.154-1	1.125-0	1.172-0	1.174-0	1.241-1	1.243-0	1.352-0	1.390-0
10	1.011-1	1.021-1	1.034-0	1.029-0	1.055-0	1.085-1	1.084-0	1.135-0	1.191-0	1.109-0	1.254-0	1.265-0	1.372-0
11	1.041-1	1.044-1	0.950-1	1.011-0	1.035-0	1.051-1	1.034-0	1.103-0	1.144-0	1.235-1	1.199-0	1.275-0	1.272-0
12	1.027-1	1.044-1	0.954-1	0.920-1	1.016-0	1.041-1	1.068-0	2.103-0	1.112-0	1.154-1	1.114-0	1.214-0	1.326-0
13	1.068-1	1.022-1	0.923-1	0.746-1	0.977-1	1.022-1	1.047-0	1.077-0	1.078-0	1.122-1	1.167-0	1.150-0	1.219-0
14	1.031-1	1.044-1	0.943-1	0.875-1	0.933-1	1.004-1	1.029-0	1.053-0	1.094-0	1.093-0	1.130-0	1.192-0	1.172-0
15	1.036-1	1.044-1	0.943-1	0.841-1	0.935-1	0.963-1	1.013-0	1.034-0	1.051-0	0.876-1	1.103-0	1.140-0	1.400-0
16	1.022-1	1.044-1	0.950-1	0.816-1	0.946-1	0.965-1	0.927-1	1.015-0	1.040-0	1.170-1	1.072-0	1.111-0	1.151-0
17	1.040-1	1.044-1	0.951-1	0.809-1	0.931-1	0.932-1	0.758-1	0.991-1	1.022-0	1.046-1	1.089-0	1.145-0	1.127-0
18	1.023-1	1.044-1	0.947-1	0.750-1	0.910-1	0.934-1	0.959-1	0.821-1	1.015-0	1.024-0	1.054-0	1.027-0	1.094-0
19	1.044-1	1.044-1	0.947-1	0.865-1	0.935-1	0.935-1	0.943-1	0.963-1	0.856-1	1.011-0	1.034-0	1.002-0	1.060-0
20	1.037-1	1.044-1	0.947-1	0.819-1	0.979-1	0.906-1	0.927-1	0.949-1	0.725-1	0.940-1	1.017-0	1.044-0	1.003-0
21	1.013-1	1.044-1	0.912-1	0.801-1	0.941-1	0.795-1	0.809-1	0.934-1	0.565-1	0.790-1	1.001-0	1.023-0	1.047-0

Table 103 (cont'd)

(V2+ MEINEL)

	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
1	1.277-0	1.253-0	1.344-0	1.195-0	1.257-0	1.452-0	1.215-0	1.227-0	1.114-0	1.236-0	1.217-0	1.244-0	1.332-0		
2	1.744-0	1.443-0	1.234-0	1.542-1	1.250-0	1.212-0	1.413-0	1.331-0	1.078-0	1.729-0	1.395-0	1.129-0	1.243-0		
3	1.734-0	1.144-0	1.572-0	1.412-0	1.334-0	1.256-0	1.214-0	1.241-0	1.524-0	1.225-0	1.214-0	1.380-1	1.443-0		
4	1.469-0	1.223-0	1.392-0	1.392-1	1.334-0	1.164-0	1.296-0	1.544-0	1.330-0	1.526-0	1.467-1	1.167-0	1.206-0		
5	1.373-0	1.213-0	1.256-0	1.256-1	1.353-0	1.374-0	1.234-0	1.093-1	1.433-0	1.136-0	1.151-1	1.454-1	1.119-0		
6	1.003-0	1.044-0	1.254-0	1.485-1	1.239-0	1.184-0	1.001-0	1.043-0	1.154-0	1.443-0	1.272-0	1.345-0	2.376-0		
7	1.773-0	1.044-0	1.555-0	1.238-0	1.178-0	1.324-0	1.196-0	1.491-1	1.372-0	1.272-0	1.174-0	1.351-0	1.314-0		
8	1.262-0	1.433-0	2.343-1	1.566-0	1.137-0	1.240-0	1.334-0	1.232-0	1.339-1	1.524-0	1.187-0	1.141-0	1.151-0		
9	1.464-0	1.574-0	1.434-0	1.704-1	1.727-0	1.450-0	1.354-0	1.011-0	1.247-0	1.152-0	1.670-0	1.244-0	1.343-1		
10	1.414-0	1.474-0	1.530-0	1.440-0	1.164-0	1.725-0	2.244-0	1.244-0	1.711-0	1.244-0	1.275-0	7.504-1	1.344-0		
11	1.413-0	1.414-0	1.444-0	1.501-0	1.372-0	1.262-0	1.814-0	5.951-1	1.731-0	1.812-0	9.756-1	1.310-0	1.281-0		
12	1.204-0	1.433-0	1.710-0	1.434-0	1.514-0	2.104-0	1.305-0	1.965-0	1.372-0	1.732-0	1.497-0	2.731-0	1.277-0		
13	1.204-0	1.433-0	1.710-0	1.434-0	1.514-0	2.104-0	1.305-0	1.965-0	2.273-0	1.494-0	1.924-0	1.481-0	1.324-0		
14	1.103-0	1.244-0	1.323-0	1.347-1	1.451-0	1.213-0	1.653-0	2.947-0	1.503-0	3.244-0	1.574-0	1.603-0	1.610-0		
15	1.103-0	1.244-0	1.323-0	1.347-1	1.451-0	1.213-0	1.653-0	2.947-0	1.553-0	1.568-0	1.628-0	1.675-0	8.393-1		
16	1.103-0	1.244-0	1.323-0	1.347-1	1.451-0	1.213-0	1.653-0	2.947-0	1.739-0	1.547-0	1.630-0	4.204-1	1.747-0		
17	1.100-0	1.244-0	1.323-0	1.292-0	1.251-0	1.331-0	1.224-0	1.491-0	1.558-0	1.743-0	7.953-1	1.702-0	1.346-0		
18	1.100-0	1.244-0	1.323-0	1.292-0	1.251-0	1.331-0	1.224-0	1.491-0	1.516-0	1.572-0	1.745-0	1.132-0	1.744-0		
19	1.100-0	1.244-0	1.323-0	1.292-0	1.251-0	1.331-0	1.224-0	1.491-0	1.239-0	1.535-0	1.544-0	1.941-0	1.306-0		
20	1.100-0	1.244-0	1.323-0	1.292-0	1.251-0	1.331-0	1.224-0	1.491-0	1.353-0	1.230-0	1.554-0	1.615-0	1.924-0		
21	1.100-0	1.244-0	1.323-0	1.292-0	1.251-0	1.331-0	1.224-0	1.491-0	1.244-0	1.374-0	1.239-0	1.574-0	1.624-0		

Table 104

R-CENTROIDS FOR (N2+ 1ST. NEC.)

	1	2	3	4	5	5	7	8	9	10
1	1.051-0	1.711-0	9.740-1	9.438-1	9.257-1	9.179-1	9.025-1	8.342-1	5.579-1	1.253-0
2	1.111-0	1.957-0	1.017-0	9.828-1	9.517-1	9.239-1	9.017-1	8.809-1	8.331-1	6.915-1
3	1.161-0	1.137-0	1.004-0	1.023-0	9.976-1	9.564-1	9.255-1	8.979-1	8.739-1	8.510-1
4	1.237-0	1.170-0	1.275-0	1.070-0	1.024-0	9.912-1	9.599-1	9.317-1	9.032-1	8.743-1
5	1.537-0	1.239-0	1.161-0	9.453-1	1.073-0	1.034-0	9.955-1	9.032-1	9.351-1	9.090-1
6	1.169-0	1.364-0	1.250-0	1.195-0	1.070-0	1.072-0	1.038-0	9.992-1	9.671-1	9.375-1
7	1.218-0	1.983-1	1.410-0	1.254-0	1.211-0	9.793-1	1.059-0	1.044-0	1.011-0	9.703-1
8	1.113-0	1.241-0	1.019-0	1.495-1	1.230-0	1.227-0	8.960-1	9.392-1	1.053-0	1.000-0
9	1.190-0	3.475-0	1.309-0	1.159-0	1.756-0	1.310-0	1.245-0	5.525-1	6.977-1	1.067-0
10	4.145-0	1.309-0	1.011-0	1.514-0	1.243-0	1.286-0	1.327-0	1.262-0	9.024-0	6.234-0
11	1.115-0	2.325-0	1.396-0	1.215-0	2.649-0	1.314-0	1.047-0	1.366-0	1.276-0	1.469-0
12	1.118-0	4.552-0	1.109-0	2.427-0	1.322-0	9.539-1	1.409-0	1.190-0	1.465-0	1.246-0
13	1.129-0	1.071-0	1.235-0	1.303-0	9.956-1	1.484-0	1.197-0	1.732-0	1.251-0	1.297-0
14	1.209-0	1.161-0	1.538-0	1.137-0	1.573-0	1.248-0	1.290-0	1.303-0	8.017-1	1.315-0
15	1.163-0	1.199-0	1.767-0	3.950-1	1.279-0	7.067-1	1.395-0	1.076-0	1.433-0	1.172-0
16	1.155-0	1.126-0	1.248-0	1.525-0	1.038-0	1.512-0	1.214-0	1.942-0	1.251-0	2.546-0
17	1.107-0	1.147-0	1.357-0	1.263-0	1.265-0	1.292-0	6.773-1	1.367-0	9.540-1	1.372-0
18	5.065-1	1.136-0	2.310-0	1.125-0	1.434-0	1.084-0	1.557-0	1.206-0	1.778-0	1.224-0
19	1.110-0	1.114-0	1.014-0	7.887-1	1.201-0	4.025-0	1.326-0	8.149-1	1.370-0	9.111-1
20	1.271-0	1.120-0	1.117-0	3.199-1	1.041-0	1.470-0	1.191-0	1.727-0	1.225-0	1.969-0
21	1.143-0	2.560-0	1.143-0	9.525-1	9.917-1	1.284-0	7.499-1	1.376-0	9.867-1	1.409-0

Table 104 (cont'd)

(N2+ 1ST. NEG.)

	11	12	13	14	15	16	17	18	19	20
1	1.113-0	1.057-0	1.078-0	1.054-0	1.035-0	9.935-1	1.594-1	1.174-0	1.163-0	1.635-0
2	9.723-1	1.521-0	4.806-0	9.975-1	1.027-0	1.214-0	9.957-1	8.201-1	1.083-0	1.046-0
3	9.132-1	9.523-1	2.679-0	1.239-0	7.732-1	9.952-1	1.022-0	1.010-0	9.113-1	1.048-0
4	9.499-1	9.253-1	7.766-1	9.125-1	7.048-1	7.126-1	7.141-1	1.047-0	1.100-0	1.193-0
5	9.803-1	8.511-1	3.223-1	7.950-1	7.238-1	4.353-1	5.591-0	1.612-0	1.243-0	1.424-0
6	9.125-1	9.453-1	8.568-1	8.213-1	7.855-1	7.459-1	6.260-1	9.653-1	1.583-0	1.260-0
7	9.725-1	9.131-1	8.875-1	9.520-1	8.246-1	7.941-1	7.277-1	6.573-1	4.523-1	7.623-1
8	9.402-1	9.414-1	9.157-1	9.885-1	9.619-1	9.341-1	7.958-1	7.397-1	5.589-1	5.742-1
9	1.0095-0	9.754-1	9.455-1	9.171-1	9.915-1	9.531-1	9.351-1	8.041-1	7.549-1	7.075-1
10	1.0000-0	9.773-1	9.825-1	9.364-1	9.175-1	8.914-1	8.559-1	8.358-1	8.083-1	7.735-1
11	1.0000-0	1.142-0	9.322-1	9.977-1	9.251-1	9.250-1	8.675-1	8.533-1	8.401-1	8.138-1
12	1.0000-0	1.733-0	1.201-0	9.153-1	1.031-0	9.951-1	9.320-1	8.797-1	8.719-1	8.424-1
13	1.0000-0	1.522-0	1.663-0	1.259-0	4.656-1	1.049-0	9.193-1	9.636-1	9.576-1	9.791-1
14	1.0000-0	1.271-0	1.484-0	1.656-0	1.344-0	1.243-0	1.159-0	6.111-1	1.018-0	8.038-1
15	1.0000-0	1.253-0	1.170-0	1.452-0	1.743-0	1.335-0	3.372-0	1.253-0	1.199-0	1.108-0
16	1.0000-0	2.027-0	1.240-0	2.570-0	1.370-0	1.895-0	1.351-0	2.302-0	1.327-0	9.655-0
17	1.0000-0	1.330-0	1.147-0	1.273-0	1.553-0	1.043-0	4.220-0	1.346-0	2.103-0	1.334-0
18	1.0000-0	1.223-0	1.459-0	1.261-0	1.133-0	1.495-0	1.615-0	1.020-0	1.365-0	2.099-0
19	1.0000-0	9.351-1	1.303-0	9.961-1	1.277-0	2.973-0	1.417-0	1.836-0	1.269-0	1.151-0
20	1.0000-0	1.524-0	1.207-0	1.397-0	1.237-0	1.253-0	1.557-0	1.954-1	2.358-0	1.332-0
21	9.706-1	1.353-0	9.106-1	1.295-0	4.716-1	1.273-0	9.392-1	1.437-0	1.329-0	9.177-1

Table 105

R-CENTROIDS FOR (V2+ 2ND. NES.)

VV	1	2	3	4	5	5	7	8	9	10
1	1.213-0	1.232-0	1.253-0	1.277-0	1.304-0	1.338-0	1.345-0	1.475-0	2.143-0	1.258-0
2	1.194-0	1.211-0	1.223-0	1.254-0	1.283-0	1.319-0	1.342-0	1.390-0	1.446-0	2.715-0
3	1.174-0	1.149-0	1.219-0	1.239-0	1.229-0	1.298-0	1.315-0	1.347-0	1.336-0	1.437-0
4	1.151-0	1.149-0	1.145-0	1.199-0	1.234-0	1.246-0	1.447-0	1.325-0	1.353-0	1.402-0
5	1.135-0	1.166-0	1.176-0	1.213-0	1.211-0	1.206-0	1.252-0	1.220-0	1.342-0	1.361-0
6	1.115-0	1.150-0	1.096-0	1.191-0	1.172-0	1.216-0	1.212-0	1.269-0	1.249-0	1.373-0
7	1.115-0	1.136-0	1.156-0	1.163-0	1.147-0	1.193-0	1.224-0	1.225-0	1.275-0	1.258-0
8	1.115-0	1.120-0	1.140-0	1.135-0	1.153-0	9.915-1	1.138-0	1.330-0	1.230-0	1.410-0
9	1.113-0	1.051-0	1.125-0	1.149-0	1.151-0	1.173-0	1.176-0	1.203-0	1.196-0	1.236-0
10	1.092-0	1.112-0	1.113-0	1.131-0	1.129-0	1.155-0	1.203-0	1.182-0	1.212-0	1.200-0
11	1.072-0	1.094-0	1.097-0	1.118-0	1.144-0	1.140-0	1.160-0	1.169-0	1.146-0	1.947-0

V	11	12	13	14	15	16	17	18	19	20
1	1.515-0	1.143-0	1.569-0	1.148-0	1.672-0	1.236-0	2.327-0	1.351-0	9.091-1	1.562-0
2	1.333-0	1.737-0	1.228-0	1.734-0	1.248-0	2.217-0	1.332-0	3.621-1	1.480-0	1.155-0
3	1.401-0	1.335-0	1.981-0	1.249-0	2.210-0	1.324-0	1.359-0	1.426-0	1.034-0	1.724-0
4	1.509-0	1.433-0	1.305-0	2.047-0	1.341-0	1.362-0	1.304-0	9.623-1	1.350-0	1.210-0
5	1.403-0	1.522-0	1.165-1	1.394-0	1.347-0	1.393-0	0.110-1	1.472-0	1.120-0	1.807-0
6	1.370-0	1.446-0	1.536-0	5.390-1	1.423-0	5.339-1	1.442-0	9.934-1	1.582-0	1.245-0
7	1.451-0	1.397-0	1.423-0	1.551-0	9.524-1	1.454-0	9.114-1	1.503-0	1.143-0	1.812-0
8	1.204-0	1.412-0	1.393-0	1.431-0	1.555-0	9.753-1	1.457-0	1.077-0	1.591-0	1.215-0
9	1.145-0	1.259-0	7.621-1	1.408-0	1.440-0	1.591-0	1.150-0	1.522-0	1.145-0	1.692-0
10	1.243-0	1.220-0	1.275-0	1.072-0	1.425-0	1.449-0	1.536-0	1.043-0	1.562-0	1.278-0
11	1.213-0	1.250-0	1.230-0	1.244-0	1.143-0	1.449-0	1.459-0	1.617-0	1.029-0	1.613-0

Table 106

D-CENTROIDS FOR (NO GAMMA (1/2))

γ	γ	1	2	3	4	5	7	8
1	1.155-0	1.041-0	1.053-0	1.034-0	1.013-0	9.942-1	9.813-1	9.475-1
2	1.155-0	1.116-0	1.066-0	1.066-0	1.045-0	1.025-0	1.016-0	9.719-1
3	1.160-0	1.145-0	1.047-0	1.047-0	1.073-0	1.053-0	1.032-0	9.944-1
4	1.200-0	1.174-0	1.126-0	1.126-0	1.137-0	1.096-0	1.054-0	1.023-0
5	1.237-0	1.210-0	1.184-0	1.148-0	1.143-0	1.115-0	1.040-0	1.050-0
6	1.278-0	1.244-0	1.215-0	1.203-0	1.158-0	1.117-0	1.115-0	1.054-0
7	1.326-0	1.245-0	1.252-0	1.223-0	1.154-0	1.167-0	1.133-0	1.097-0
8	1.377-0	1.331-0	1.242-0	1.259-0	1.232-0	1.191-0	1.179-0	1.144-0
9	1.440-0	1.379-0	1.337-0	1.293-0	1.266-0	1.244-0	1.203-0	1.154-0
10	1.420-0	1.421-0	1.335-0	1.343-0	1.316-0	1.273-0	1.240-0	1.135-0
11	1.474-0	1.459-0	1.422-0	1.347-0	1.344-0	1.312-0	1.241-0	1.223-0
12	1.501-0	1.432-0	1.439-0	1.421-0	1.390-0	1.354-0	1.319-0	1.251-0
13	1.415-0	1.354-0	1.443-0	1.439-0	1.424-0	1.395-0	1.350-0	1.294-0
14	1.132-0	1.319-0	1.448-0	1.459-0	1.449-0	1.430-0	1.400-0	1.333-0
15	1.232-1	1.249-0	1.657-1	1.591-0	1.449-0	1.461-0	1.436-0	1.373-0
16	1.212-0	1.136-0	1.254-0	1.617-0	1.652-0	1.513-0	1.470-0	1.413-0
			1.131-0	1.172-0	2.339-0	1.517-0	1.517-0	1.451-0

Table 106 (cont'd)

(10 GAYNA(1/2))

	9	10	11	12	13	14	15	16	17
1	3.315-1	3.163-1	9.121-1	3.893-1	3.752-1	3.635-1	3.515-1	3.359-1	3.161-1
2	3.540-1	3.348-1	9.236-1	3.909-1	3.933-1	3.824-1	3.695-1	3.523-1	3.358-1
3	3.777-1	3.515-1	9.400-1	3.931-1	3.953-1	3.813-1	3.678-1	3.477-1	3.291-1
4	3.992-1	3.647-1	9.544-1	3.952-1	3.979-1	3.834-1	3.691-1	3.455-1	3.236-1
5	4.194-1	3.759-1	9.613-1	3.975-1	3.997-1	3.847-1	3.701-1	3.419-1	3.199-1
6	4.385-1	3.937-1	9.707-1	3.998-1	3.825-1	3.658-1	3.516-1	3.270-1	3.028-1
7	4.564-1	4.040-1	9.798-1	4.025-1	3.916-1	3.696-1	3.739-1	3.588-1	3.442-1
8	4.732-1	4.169-1	9.869-1	4.031-1	3.939-1	3.714-1	3.959-1	3.810-1	3.659-1
9	4.889-1	4.231-1	9.922-1	4.069-1	3.944-1	3.914-1	3.924-1	3.805-1	3.644-1
10	5.034-1	4.232-1	9.966-1	4.104-1	3.978-1	3.958-1	3.938-1	3.847-1	3.713-1
11	5.168-1	4.240-1	1.044-1	4.109-1	3.975-1	3.989-1	3.967-1	3.849-1	3.730-1
12	5.292-1	4.249-1	1.022-1	4.155-1	3.924-1	3.956-1	3.935-1	3.778-1	3.658-1
13	5.415-1	4.271-1	1.030-1	4.149-1	3.968-1	3.935-1	3.903-1	3.751-1	3.691-1
14	5.534-1	4.311-1	1.027-1	4.220-1	3.941-1	3.989-1	3.948-1	3.719-1	3.659-1
15	5.641-1	4.351-1	1.027-1	4.243-1	3.934-1	3.997-1	3.973-1	3.761-1	3.732-1
16	5.741-1	4.351-1	1.034-1	4.244-1	3.963-1	3.948-1	3.912-1	3.760-1	3.743-1
17	5.822-1	4.392-1	1.037-1	4.304-1	3.978-1	3.974-1	3.955-1	3.826-1	3.799-1

Table 107

R-CENTROIDS FOR (NO GAMMA (3/2))

ν	VV	0	1	2	3	4	5	7	8
0	1.113-0	1.093-0	1.075-0	1.054-0	1.041-0	1.026-0	1.012-0	9.987-1	9.859-1
1	1.134-0	1.115-0	1.087-0	1.085-0	1.055-0	1.048-0	1.032-0	1.018-0	1.014-0
2	1.154-0	9.435-1	1.123-0	1.111-0	1.079-0	1.087-0	1.056-0	1.039-0	1.024-0
3	1.175-0	1.173-0	1.144-0	1.134-0	1.103-0	1.088-0	1.057-0	1.042-0	1.044-0
4	1.225-0	1.218-0	1.210-0	1.153-0	1.124-0	1.126-0	1.096-0	1.076-0	1.056-0
5	1.250-0	1.231-0	1.219-0	1.171-0	1.154-0	1.135-0	1.100-0	1.109-0	1.094-0
6	1.301-0	1.266-0	1.234-0	1.221-0	1.143-0	1.216-0	1.144-0	1.119-0	9.795-1
7	1.345-0	1.306-0	1.273-0	1.246-0	1.447-0	1.193-0	1.151-0	1.156-0	1.127-0
8	1.390-0	1.349-0	1.312-0	1.279-0	1.254-0	1.210-0	1.203-0	1.168-0	1.212-0
9	1.423-0	1.394-0	1.355-0	1.314-0	1.236-0	1.264-0	1.224-0	1.219-0	1.179-0
10	1.544-0	1.431-0	1.396-0	1.359-0	1.323-0	1.293-0	1.287-0	1.234-0	1.213-0
11	1.547-0	1.450-0	1.426-0	1.394-0	1.364-0	1.329-0	1.300-0	1.247-0	1.244-0
12	1.274-0	1.425-0	1.444-0	1.429-0	1.413-0	1.359-0	1.336-0	1.308-0	1.253-0
13	1.318-0	1.411-0	1.471-0	1.457-0	1.436-0	1.408-0	1.375-0	1.343-0	1.317-0
14	1.210-0	1.164-0	1.715-0	1.515-0	1.470-0	1.443-0	1.414-0	1.381-0	1.350-0
15	1.429-0	1.251-0	1.179-0	1.829-0	1.535-0	1.480-0	1.450-0	1.420-0	1.338-0
16	1.205-0	1.197-0	1.241-0	1.793-0	1.652-0	1.535-0	1.498-0	1.457-0	1.429-0

Table 107 (cont'd)

(NO GA44A(3/2))

	VV	9	10	11	12	13	14	15	16	17
1	9.730-1	9.619-1	9.508-1	9.433-1	9.373-1	9.267-1	9.114-1	9.019-1	9.913-1	
2	9.915-1	9.743-1	9.656-1	9.565-1	9.458-1	9.355-1	9.257-1	9.161-1	9.064-1	
3	1.011-0	9.972-1	9.849-1	9.733-1	9.622-1	9.514-1	9.410-1	9.309-1	9.210-1	
4	1.051-0	1.016-0	1.013-1	9.937-1	9.739-1	9.577-1	9.370-1	9.166-1	8.964-1	
5	7.791-1	1.041-0	1.023-1	1.009-0	9.906-1	9.845-1	9.732-1	9.624-1	9.521-1	
6	1.006-0	1.047-0	9.311-1	1.033-0	1.016-0	1.013-0	9.936-1	9.790-1	9.641-1	
7	1.094-0	1.074-0	1.050-0	1.034-0	9.360-1	1.026-0	1.010-0	9.967-1	9.853-1	
8	1.100-0	1.127-0	1.093-0	1.064-0	1.049-0	1.031-0	9.069-1	1.014-0	1.003-0	
9	1.136-0	1.111-0	1.079-0	1.100-0	1.073-0	1.056-0	1.041-0	1.025-0	7.805-1	
10	1.135-0	1.150-0	1.121-0	1.097-0	1.024-0	1.086-0	1.055-0	1.049-0	1.035-0	
11	1.140-0	1.157-0	1.209-0	1.132-0	1.108-0	1.083-0	1.177-0	1.076-0	1.058-0	
12	1.200-0	1.204-0	1.169-0	1.125-0	1.148-0	1.118-0	1.036-0	1.066-0	1.103-0	
13	1.254-0	1.217-0	1.232-0	1.191-0	1.149-0	1.234-0	1.131-0	1.107-0	1.045-0	
14	1.240-0	1.258-0	1.230-0	1.179-0	1.193-0	1.162-0	1.121-0	1.151-0	1.119-0	
15	1.343-0	1.248-0	1.330-0	1.242-0	1.200-0	1.215-0	1.173-0	1.143-0	1.133-0	
16	1.354-0	1.299-0	1.293-0	1.259-0	1.255-0	1.220-0	1.393-0	1.198-0	1.156-0	
17	1.598-0	1.374-0	1.298-0	1.293-0	1.243-0	1.266-0	1.235-0	1.140-0	1.210-0	

Table 108

P-CENTROIDS FOR (NO BETA)

V	VV	1	2	3	4	5	6	7	8
1	1.270-0	1.246-0	1.313-1	1.320-0	1.337-1	1.355-0	1.373-0	1.393-0	1.412-0
2	1.261-0	1.277-0	1.293-1	1.319-0	1.326-0	1.344-0	1.361-0	1.379-0	1.395-0
3	1.252-0	1.264-0	1.274-0	1.290-0	1.316-0	1.333-0	1.348-0	1.368-0	1.383-0
4	1.244-0	1.259-0	1.274-1	1.290-0	1.316-0	1.320-0	1.349-0	1.360-0	1.376-0
5	1.230-0	1.251-0	1.266-1	1.291-0	1.295-1	1.326-0	1.332-0	1.347-0	1.353-0
6	1.220-0	1.242-0	1.257-1	1.272-0	1.273-1	1.307-0	1.321-0	1.333-0	1.363-0
7	1.213-0	1.234-0	1.249-1	1.262-0	1.293-0	1.296-0	1.309-0	1.335-0	1.346-0
8	1.205-0	1.227-0	1.241-1	1.243-0	1.273-0	1.286-0	1.412-0	1.321-0	1.334-0
9	1.193-0	1.219-0	1.232-1	1.253-0	1.264-0	1.275-0	1.298-0	1.310-0	1.313-0
10	1.182-0	1.212-0	1.223-1	1.243-0	1.255-1	1.320-0	1.247-0	1.299-0	1.322-0
11	1.172-0	1.205-0	1.219-1	1.235-0	1.246-0	1.257-0	1.277-0	1.454-0	1.310-0
12	1.160-0	1.198-0	1.219-1	1.227-0	1.233-0	1.257-0	1.257-0	1.289-0	1.300-0
13	1.145-0	1.181-0	1.209-1	1.220-0	1.247-0	1.248-0	1.248-0	1.279-0	1.298-0
14	1.130-0	1.170-0	1.201-1	1.212-0	1.231-0	1.240-0	1.255-0	1.270-0	1.354-0
15	1.115-0	1.154-0	1.194-1	1.205-0	1.223-0	1.232-0	1.252-0	1.260-1	1.292-0
16	1.105-0	1.144-0	1.182-1	1.193-0	1.216-0	1.219-0	1.243-0	1.247-0	1.272-0
17	1.144-0	1.160-0	1.176-1	1.191-0	1.219-0	1.238-0	1.235-0	1.279-0	1.263-0
18	1.143-0	1.154-0	1.170-1	1.184-0	1.216-0	1.220-0	1.228-0	1.248-0	1.254-0
19	1.143-0	1.154-0	1.170-1	1.184-0	1.216-0	1.212-0	1.220-0	1.239-0	1.243-0

(AND BETA)

Table 108 (cont'd)

VV	9	10	11	12	13	14	15	16
V								
1	1.412-0	1.433-0	1.454-0	1.475-0	1.496-0	1.517-0	1.538-0	1.559-0
2	1.435-0	1.456-0	1.477-0	1.498-0	1.519-0	1.540-0	1.561-0	1.582-0
3	1.458-0	1.479-0	1.500-0	1.521-0	1.542-0	1.563-0	1.584-0	1.605-0
4	1.481-0	1.502-0	1.523-0	1.544-0	1.565-0	1.586-0	1.607-0	1.628-0
5	1.504-0	1.525-0	1.546-0	1.567-0	1.588-0	1.609-0	1.630-0	1.651-0
6	1.527-0	1.548-0	1.569-0	1.590-0	1.611-0	1.632-0	1.653-0	1.674-0
7	1.550-0	1.571-0	1.592-0	1.613-0	1.634-0	1.655-0	1.676-0	1.697-0
8	1.573-0	1.594-0	1.615-0	1.636-0	1.657-0	1.678-0	1.699-0	1.720-0
9	1.596-0	1.617-0	1.638-0	1.659-0	1.680-0	1.701-0	1.722-0	1.743-0
10	1.619-0	1.640-0	1.661-0	1.682-0	1.703-0	1.724-0	1.745-0	1.766-0
11	1.642-0	1.663-0	1.684-0	1.705-0	1.726-0	1.747-0	1.768-0	1.789-0
12	1.665-0	1.686-0	1.707-0	1.728-0	1.749-0	1.770-0	1.791-0	1.812-0
13	1.688-0	1.709-0	1.730-0	1.751-0	1.772-0	1.793-0	1.814-0	1.835-0
14	1.711-0	1.732-0	1.753-0	1.774-0	1.795-0	1.816-0	1.837-0	1.858-0
15	1.734-0	1.755-0	1.776-0	1.797-0	1.818-0	1.839-0	1.860-0	1.881-0
16	1.757-0	1.778-0	1.799-0	1.820-0	1.841-0	1.862-0	1.883-0	1.904-0
17	1.780-0	1.801-0	1.822-0	1.843-0	1.864-0	1.885-0	1.906-0	1.927-0
18	1.803-0	1.824-0	1.845-0	1.866-0	1.887-0	1.908-0	1.929-0	1.950-0

Table 109

R-CENTROIDS FOR (NO DELTA (1/2))

VV	1	2	3	4	5	6	7	8	9	10	11
1	1.112-1	1.067-1	1.043-1	1.031-1	1.014-1	0.975-1	0.917-1	0.841-1	0.754-1	0.273-1	0.174-1
2	1.137-1	1.125-1	1.070-1	1.055-1	1.037-1	1.020-1	1.004-1	0.979-1	0.713-1	0.543-1	0.365-1
3	1.157-1	1.120-1	1.095-1	1.104-1	1.083-1	1.043-1	1.025-1	1.010-1	0.930-1	0.779-1	0.620-1
4	1.177-1	1.134-1	1.131-1	1.114-1	1.080-1	1.048-1	1.031-1	1.032-1	1.015-1	0.939-1	0.844-1
5	1.211-1	1.191-1	1.149-1	1.170-1	1.113-1	1.090-1	1.055-1	1.063-1	1.039-1	1.021-1	1.005-1
1	0.804-1	0.583-1	0.124-1	0.133-1	0.343-1	0.359-1	0.752-1	0.770-1	0.922-1	1.004-1	1.011-1
2	0.115-1	0.093-1	0.530-1	0.244-1	0.246-1	0.131-1	1.122-1	1.058-1	1.014-1	0.955-1	0.599-1
3	0.400-1	0.281-1	0.336-1	0.511-1	0.445-1	0.559-1	0.621-1	1.233-1	1.069-1	1.011-1	0.787-1
4	0.614-1	0.513-1	0.145-1	0.907-1	0.532-1	0.053-1	0.931-1	1.065-1	1.397-1	1.032-1	1.016-1
5	0.893-1	0.744-1	0.500-1	0.211-1	0.491-1	0.714-1	0.204-1	0.439-1	3.749-1	1.604-1	1.143-1

Table II0

R-CENTROIDS FOR (NO JELIA (3/2))

V	VV	1	2	3	4	5	6	7	8	9	10	11
1	1.13-1	1.081-0	1.068-0	1.050-0	1.033-0	1.017-0	1.001-0	0.984-1	0.968-1	0.952-1	0.936-1	0.920-1
2	1.137-1	1.111-0	1.135-0	1.177-0	1.237-0	1.319-0	1.423-0	1.557-0	1.719-0	1.908-0	2.121-0	2.357-0
3	1.137-0	1.134-0	1.121-0	1.096-0	1.066-0	1.035-0	1.005-0	0.978-0	0.952-0	0.928-0	0.905-0	0.883-0
4	1.211-0	1.177-0	1.135-0	1.083-0	1.035-0	0.992-0	0.954-0	0.921-0	0.893-0	0.868-0	0.845-0	0.823-0
5	1.240-0	1.211-0	1.192-0	1.149-0	1.095-0	1.038-0	0.981-0	0.928-0	0.880-0	0.837-0	0.799-0	0.766-0
6	1.273-1	1.243-1	1.206-1	1.149-1	1.083-1	1.017-1	0.952-1	0.888-1	0.828-1	0.773-1	0.723-1	0.678-1
7	1.310-1	1.279-1	1.239-1	1.179-1	1.113-1	1.047-1	0.982-1	0.918-1	0.858-1	0.803-1	0.753-1	0.708-1
8	1.351-1	1.319-1	1.278-1	1.216-1	1.149-1	1.083-1	1.018-1	0.954-1	0.894-1	0.839-1	0.789-1	0.744-1
9	1.396-1	1.363-1	1.321-1	1.257-1	1.190-1	1.124-1	1.059-1	0.995-1	0.936-1	0.881-1	0.831-1	0.786-1
10	1.445-1	1.411-1	1.368-1	1.303-1	1.236-1	1.169-1	1.104-1	1.040-1	0.981-1	0.927-1	0.877-1	0.832-1
11	1.498-1	1.463-1	1.419-1	1.353-1	1.286-1	1.219-1	1.154-1	1.090-1	1.031-1	0.977-1	0.927-1	0.882-1
12	1.555-1	1.519-1	1.475-1	1.409-1	1.342-1	1.275-1	1.210-1	1.146-1	1.087-1	1.033-1	0.983-1	0.938-1
13	1.617-1	1.581-1	1.537-1	1.471-1	1.404-1	1.337-1	1.272-1	1.208-1	1.149-1	1.095-1	1.045-1	1.000-1
14	1.684-1	1.647-1	1.603-1	1.537-1	1.470-1	1.403-1	1.338-1	1.274-1	1.215-1	1.161-1	1.111-1	1.066-1
15	1.756-1	1.719-1	1.675-1	1.609-1	1.542-1	1.475-1	1.410-1	1.346-1	1.287-1	1.233-1	1.183-1	1.138-1
16	1.833-1	1.796-1	1.752-1	1.686-1	1.619-1	1.552-1	1.487-1	1.423-1	1.364-1	1.310-1	1.260-1	1.215-1
17	1.915-1	1.878-1	1.834-1	1.768-1	1.701-1	1.634-1	1.569-1	1.505-1	1.446-1	1.392-1	1.342-1	1.297-1
18	2.002-1	1.965-1	1.921-1	1.855-1	1.788-1	1.721-1	1.656-1	1.592-1	1.533-1	1.479-1	1.429-1	1.384-1
19	2.094-1	2.057-1	2.013-1	1.947-1	1.880-1	1.813-1	1.748-1	1.684-1	1.625-1	1.571-1	1.521-1	1.476-1
20	2.191-1	2.154-1	2.110-1	2.044-1	1.977-1	1.910-1	1.845-1	1.781-1	1.722-1	1.668-1	1.618-1	1.573-1
21	2.293-1	2.256-1	2.212-1	2.146-1	2.079-1	2.012-1	1.947-1	1.883-1	1.824-1	1.770-1	1.720-1	1.675-1
22	2.400-1	2.363-1	2.319-1	2.253-1	2.186-1	2.119-1	2.054-1	1.990-1	1.931-1	1.877-1	1.827-1	1.782-1
23	2.512-1	2.475-1	2.431-1	2.365-1	2.298-1	2.231-1	2.166-1	2.102-1	2.043-1	1.989-1	1.939-1	1.894-1

Table III

R-CENTROIDS FOR (NO EPSILON (1/2))

VV	1	2	3	4	5	6	7	8	9	10	11
1	1.119-0	1.096-0	1.044-0	1.033-0	1.115-0	1.039-1	1.052-1	9.731-1	9.502-1	9.459-1	9.327-1
2	1.116-0	1.159-0	1.170-0	1.055-0	1.137-0	1.020-0	1.005-0	9.909-1	9.773-1	9.542-1	9.517-1
3	1.110-0	1.118-0	1.132-0	1.120-0	1.105-0	1.043-0	1.028-0	1.011-0	9.951-1	9.326-1	9.599-1
4	1.114-0	1.144-0	1.131-0	1.102-0	1.170-0	1.112-0	1.054-0	1.033-0	1.117-0	1.012-0	9.482-1
5	1.234-0	1.142-0	1.152-0	1.040-0	1.113-0	1.040-0	1.032-0	9.797-1	1.144-0	1.024-0	1.004-0
6	1.270-0	1.211-0	1.107-0	1.152-0	1.129-0	1.134-0	1.027-0	1.072-0	1.149-0	1.170-0	1.133-0
7	1.312-0	1.244-0	1.210-0	1.133-0	1.172-0	1.144-0	1.069-0	1.115-0	1.184-0	1.161-0	1.139-0
7	1.311-0	1.278-0	1.250-0	1.215-0	1.201-0	1.142-0	1.155-0	1.126-0	1.142-0	1.100-0	1.073-0

VV	12	13	14	15	16	17	18	19	20	21	22	23
1	9.172-1	9.030-1	9.334-1	9.023-1	8.859-1	9.344-1	9.384-1	9.720-1	8.043-1	1.105-0	1.050-0	1.032-0
2	9.315-1	9.270-1	9.157-1	9.132-1	8.848-1	8.599-1	9.411-1	7.957-1	6.145-1	2.453-0	1.143-0	1.020-0
3	9.574-1	9.452-1	9.328-1	9.134-1	9.354-1	8.447-1	9.532-1	9.471-1	7.928-1	6.577-1	9.263-1	1.153-0
4	9.700-1	9.520-1	9.437-1	9.371-1	9.243-1	9.003-1	9.348-1	9.754-1	8.479-1	7.935-1	6.566-1	3.104-0
5	9.936-1	9.403-1	9.575-1	9.550-1	9.424-1	9.295-1	9.159-1	9.015-1	8.909-1	8.514-1	7.945-1	0.124-1
6	1.010-0	1.001-0	9.861-1	9.732-1	9.609-1	9.484-1	9.352-1	9.217-1	9.043-1	8.442-1	8.553-1	8.700-1
7	1.031-0	1.024-0	1.019-0	9.934-1	9.745-1	9.604-1	9.540-1	9.417-1	9.271-1	9.133-1	8.839-1	9.591-1
7	1.031-0	1.025-0	1.033-0	1.115-0	1.031-0	9.473-1	9.734-1	9.508-1	9.466-1	9.334-1	9.193-1	8.989-1

Table II2

P-CENTROIDS FOR (NO EPSILON (3/2))

V	VV	1	2	3	4	5	6	7	8	9	10	11
1	1.119-0	1.084-0	1.064-0	1.050-0	1.033-0	1.017-0	1.003-0	0.891-1	9.741-1	9.510-1	9.479-1	9.365-1
2	1.135-0	1.110-0	0.453-1	1.077-0	1.056-0	1.039-0	1.023-0	1.004-0	9.935-1	9.410-1	9.571-1	9.543-1
3	1.150-0	1.150-0	1.119-0	1.033-0	1.052-0	1.067-0	1.045-0	1.028-0	1.013-0	9.987-1	9.953-1	9.723-1
4	1.165-0	1.175-0	1.146-0	1.135-0	1.103-0	1.079-0	1.039-0	1.037-0	1.035-0	1.019-0	1.004-0	9.905-1
5	1.253-0	1.204-0	1.183-0	1.152-0	1.096-0	1.114-0	1.037-0	1.034-0	1.019-0	1.045-0	1.026-0	1.010-0
6	1.259-0	1.239-0	1.210-0	1.173-0	1.152-0	1.131-0	1.152-0	1.000-0	1.074-0	1.052-0	9.238-1	1.035-0
7	1.303-0	1.274-0	1.243-0	1.214-0	1.192-0	1.173-0	1.145-0	1.101-0	1.119-0	1.086-0	1.063-0	1.042-0
8	1.325-0	1.305-0	1.277-0	1.249-0	1.212-0	1.201-0	1.205-0	1.157-0	1.129-0	1.092-0	1.123-0	1.075-0

V	VV	12	13	14	15	16	17	18	19	20	21	22	23
1	9.204-1	9.171-1	9.068-1	8.924-1	8.693-1	8.220-1	7.031-1	1.020-0	1.551-0	1.132-0	1.008-0	9.361-1	
2	9.444-1	9.290-1	9.173-1	9.043-1	8.913-1	8.745-1	8.494-1	8.018-1	6.444-1	2.557-0	1.140-0	1.034-0	
3	9.545-1	9.471-1	9.345-1	9.219-1	9.089-1	8.944-1	8.765-1	8.519-1	8.036-1	6.590-1	3.465-0	1.142-0	
4	9.775-1	9.643-1	9.524-1	9.394-1	9.268-1	9.132-1	8.977-1	8.757-1	8.520-1	8.042-1	6.667-1	4.331-0	
5	9.911-1	9.828-1	9.703-1	9.578-1	9.452-1	9.319-1	9.178-1	8.922-1	8.832-1	8.562-1	8.074-1	6.525-1	
6	1.013-0	1.003-0	9.847-1	9.757-1	9.633-1	9.510-1	9.379-1	9.235-1	9.074-1	8.479-1	8.606-1	6.115-1	
7	1.055-0	1.025-0	1.010-0	9.959-1	9.822-1	9.690-1	9.555-1	9.441-1	9.375-1	9.142-1	8.934-1	8.641-1	
8	1.093-0	1.033-0	1.034-0	1.015-0	1.003-0	9.901-1	9.764-1	9.629-1	9.496-1	9.363-1	9.215-1	9.024-1	

Table III3

2-CENTROIDS FOR (NO BETA PRIME (1/2))

VV	1	2	3	4	5	6	7	8	9	10	11
1	1.222-0	1.277-0	1.230-0	1.321-0	1.344-0	1.376-0	1.416-0	1.433-0	1.464-0	1.499-0	1.529-0
2	1.227-0	1.254-0	1.270-0	1.311-0	1.332-0	1.359-0	1.385-0	1.413-0	1.443-0	1.473-0	1.505-0
3	1.192-0	1.230-0	1.260-0	1.248-0	1.311-0	1.415-0	1.750-0	1.335-0	1.423-0	1.452-0	1.483-0
4	1.173-0	1.228-0	1.244-0	1.259-0	1.332-0	1.323-0	1.346-0	1.469-0	1.436-0	1.473-0	1.462-0
5	1.154-0	1.211-0	1.235-0	1.205-0	1.252-0	1.321-0	1.337-0	1.359-0	1.391-0	1.433-0	1.444-0
6	1.151-0	1.148-0	1.212-0	1.245-0	1.204-0	1.290-0	1.315-0	1.331-0	1.371-0	1.394-0	1.416-0

VV	12	13	14	15	16	17	18	19	20	21	22	23
1	1.220-0	1.434-0	2.049-0	1.434-0	1.344-0	1.343-0	1.355-0	1.352-0	1.438-0	1.365-0	1.294-0	1.406-0
2	1.542-0	1.573-0	1.607-0	1.617-0	1.617-0	1.219-0	1.340-0	1.421-0	1.396-0	1.379-0	1.344-0	1.359-0
3	1.510-0	1.551-0	1.544-0	1.604-0	1.654-0	1.419-0	1.997-0	1.555-0	1.542-0	1.365-0	1.515-0	1.479-0
4	1.413-0	1.524-0	1.527-0	1.531-0	1.629-0	1.581-0	1.736-0	1.751-0	1.672-0	1.531-0	1.437-0	1.424-0
5	1.472-0	1.592-0	1.534-0	1.554-0	1.644-0	1.640-0	1.549-0	1.751-0	1.711-0	1.752-0	3.534-0	1.275-0
6	1.444-0	1.445-0	1.513-0	1.544-0	1.574-0	1.614-0	1.650-0	1.622-0	1.731-0	1.745-0	1.424-0	1.325-0

NOT REPRODUCIBLE

Table II4

R-CENTROIDS FOR (NO BETA PRIME (3/2))

VV	1	2	3	4	5	6	7	8	9	10	11
1	1.247-0	1.272-0	1.297-0	1.323-0	1.349-0	1.377-0	1.405-0	1.436-0	1.465-0	1.494-0	1.531-0
2	1.231-0	1.255-0	1.277-0	1.311-0	1.333-0	1.359-0	1.387-0	1.415-0	1.444-0	1.474-0	1.507-0
3	1.215-0	1.236-0	1.257-0	1.249-0	1.312-0	1.357-0	1.371-0	1.336-0	1.424-0	1.454-0	1.485-0
4	1.212-0	1.229-0	1.251-0	1.269-0	1.303-0	1.324-0	1.348-0	1.412-0	1.434-0	1.435-0	1.464-0
5	1.181-0	1.212-0	1.234-0	1.264-0	1.283-0	1.332-0	1.337-0	1.359-0	1.392-0	1.439-0	1.446-0
6	1.171-0	1.193-0	1.194-0	1.246-0	1.264-0	1.297-0	1.316-0	1.333-0	1.372-0	1.396-0	1.416-0

VV	12	13	14	15	16	17	18	19	20	21	22	23
1	1.036-0	1.051-0	1.077-0	1.047-0	1.295-0	1.314-0	1.375-0	1.675-0	1.393-0	1.203-0	1.396-0	1.324-0
2	1.032-0	1.039-0	1.033-0	1.563-0	1.945-0	1.237-0	1.328-0	1.428-0	1.334-0	1.585-0	1.421-0	5.771-1
3	1.017-0	1.051-0	1.037-0	1.619-0	1.637-0	1.793-0	5.474-0	1.484-0	1.527-0	1.279-0	1.328-0	1.397-0
4	1.034-0	1.052-0	1.060-0	1.595-0	1.630-0	1.065-0	1.741-0	2.091-0	1.539-0	1.547-0	9.705-1	1.253-0
5	1.044-0	1.051-0	1.036-0	1.570-0	1.605-0	1.041-0	1.686-0	1.751-0	1.798-0	1.640-0	1.607-0	1.391-0
6	1.031-0	1.046-0	1.015-0	1.549-0	1.590-0	1.016-0	1.693-0	1.695-0	1.733-0	1.739-0	1.755-0	7.977-0

NOT REPRODUCIBLE

Table II5

P-CENTROIDS FOR (N) GAMMA PRIME)

VV	1	2	3	4	5	6	7	8	9	10	11
1	1.087-0	1.057-0	1.044-0	1.031-0	1.014-0	0.973-1	0.924-1	0.872-1	0.824-1	0.741-1	0.647-1
2	1.110-0	1.136-0	1.170-0	1.055-0	1.037-0	1.020-0	1.014-0	0.972-1	0.943-1	0.833-1	0.743-1
3	1.100-0	1.120-0	1.130-0	1.031-0	1.005-0	1.014-0	1.027-0	1.011-0	0.935-1	0.810-1	0.674-1
4	1.100-0	1.141-0	1.143-0	1.124-0	1.031-0	1.026-0	1.054-0	1.034-0	1.017-0	1.002-0	0.940-1
5	1.224-0	1.145-0	1.150-0	1.115-0	1.113-0	1.030-0	1.057-0	0.974-1	1.045-0	1.025-0	1.009-0
6	1.200-0	1.211-0	1.075-0	1.157-0	1.130-0	1.129-0	1.000-0	1.076-0	1.053-0	0.910-0	1.035-0

VV	12	13	14	15	16	17	18	19	20	21	22	23
1	0.117-1	0.030-1	0.998-1	0.002-1	0.068-1	0.151-1	0.157-1	0.041-1	0.004-1	1.302-0	1.103-0	1.072-0
2	0.538-1	0.234-1	0.153-1	0.091-1	0.029-1	0.336-1	0.771-1	0.472-1	0.901-1	0.587-1	1.124-0	1.023-0
3	0.544-1	0.422-1	0.303-1	0.187-1	0.074-1	0.465-1	0.851-1	0.748-1	0.606-1	0.399-1	0.066-1	0.475-1
4	0.741-1	0.600-1	0.477-1	0.356-1	0.240-1	0.125-1	0.012-1	0.059-1	0.799-1	0.579-1	0.550-1	0.365-1
5	0.942-1	0.400-1	0.672-1	0.541-1	0.416-1	0.299-1	0.199-1	0.001-1	0.959-1	0.847-1	0.716-1	0.574-1
6	1.000-0	0.000-0	0.405-1	0.733-1	0.612-1	0.406-1	0.353-1	0.215-1	0.134-1	0.128-1	0.922-1	0.909-1

NOT REPRODUCIBLE

Table II6 P-CENTROIDS FOR (NO FEAST 1)

VV	1	2	3	4	5
0	1.0066-0	9.313-1	9.5-7-1	1.175-0	1.039-0
1	3.927-0	9.910-1	9.051-1	4.702-1	1.114-0
2	1.162-0	5.024-0	9.943-1	9.279-1	9.426-1
3	9.140-1	1.230-0	1.141-0	3.856-0	8.150-1
4	1.196-0	3.823-1	1.353-0	1.150-0	2.941-1
5	1.635-0	1.034-0	1.129-0	1.300-0	1.110-0
6	9.532-1	9.457-1	2.135-0	2.179-0	1.330-0
7	9.570-1	9.608-1	9.224-1	3.042-0	8.520-1

Table II7 R-CENTROIDS FOR (NO FEAST 2)

VV	1	2	3	4	5
0	1.683-0	1.074-0	9.352-1	1.124-0	1.034-0
1	1.076-0	1.987-0	1.037-0	1.093-0	1.097-0
2	3.297-1	1.034-0	1.872-0	1.173-0	1.246-0
3	5.146-0	3.041-1	1.032-0	1.620-0	1.127-0
4	1.259-0	1.419-1	3.625-1	1.100-0	1.957-0
5	1.009-0	3.203-0	1.307-1	3.306-1	1.109-0

NOT REPRODUCIBLE

Table II8

R-CENTROIDS FOR (NO FEAST HEAT)							
VV	1	2	3	4	5	6	7
1	1.003-0	1.235-0	1.155-0	1.135-0	1.154-0	2.152-0	1.075-0
2	1.003-1	1.723-0	1.094-0	1.323-0	1.123-0	1.130-0	1.163-0
3	1.003-1	1.044-0	1.093-0	1.144-0	1.094-0	1.112-0	2.745-0
4	1.003-1	2.053-1	1.093-0	2.078-0	1.212-0	1.369-1	1.067-0
5	1.003-1	1.143-1	1.221-1	1.102-0	2.303-0	1.574-0	1.229-0
6	1.003-1	0.174-1	0.444-1	0.665-1	1.110-0	2.712-0	0.461-1

Table II9

R-CENTROIDS FOR (NO L-M)										
VV	1	2	3	4	5	6	7	8	9	10
1	1.204-0	1.246-0	1.304-0	1.330-0	1.353-0	1.377-0	1.411-0	1.430-0	1.452-0	1.479-0
2	1.204-0	1.273-0	1.294-0	1.315-0	1.321-0	1.355-0	1.387-0	1.411-0	1.436-0	1.461-0
3	1.204-0	1.260-0	1.281-0	1.310-0	1.327-0	1.348-0	1.359-0	1.405-0	1.422-0	1.446-0
4	1.204-0	1.248-0	1.270-0	1.292-0	1.312-0	1.312-0	1.350-0	1.381-0	1.412-0	1.504-0
5	1.204-0	1.234-0	1.259-0	1.279-0	1.274-0	1.324-0	1.343-0	1.357-0	1.393-0	1.415-0
6	1.204-0	1.227-0	1.247-0	1.265-0	1.291-0	1.310-0	1.317-0	1.356-0	1.375-0	1.397-0
7	1.204-0	1.216-0	1.235-0	1.259-0	1.274-0	1.293-0	1.324-0	1.340-0	1.314-0	1.344-0
8	1.204-0	1.205-0	1.222-0	1.246-0	1.266-0	1.291-0	1.319-0	1.316-0	1.354-0	1.371-0
9	1.204-0	1.204-0	1.222-0	1.246-0	1.266-0	1.291-0	1.319-0	1.316-0	1.354-0	1.371-0
10	1.204-0	1.204-0	1.222-0	1.246-0	1.266-0	1.291-0	1.319-0	1.316-0	1.354-0	1.371-0
11	1.204-0	1.204-0	1.222-0	1.246-0	1.266-0	1.291-0	1.319-0	1.316-0	1.354-0	1.371-0

R-CENTROIDS FOR (NO L-M)										
VV	12	13	14	15	16	17	18	19	20	21
1	1.532-0	1.564-0	1.577-0	1.524-0	1.577-0	1.743-0	1.530-0	1.258-0	1.427-0	1.241-0
2	1.532-0	1.543-0	1.577-0	1.513-0	1.540-0	1.540-0	1.735-0	1.615-0	1.657-0	1.513-0
3	1.532-0	1.543-0	1.577-0	1.513-0	1.540-0	1.540-0	1.592-0	1.775-0	1.858-0	1.565-0
4	1.532-0	1.543-0	1.577-0	1.513-0	1.540-0	1.540-0	1.592-0	1.690-0	1.731-0	1.799-0
5	1.532-0	1.543-0	1.577-0	1.513-0	1.540-0	1.540-0	1.592-0	1.672-0	1.709-0	1.753-0
6	1.532-0	1.543-0	1.577-0	1.513-0	1.540-0	1.540-0	1.592-0	1.672-0	1.709-0	1.753-0
7	1.532-0	1.543-0	1.577-0	1.513-0	1.540-0	1.540-0	1.592-0	1.672-0	1.709-0	1.753-0
8	1.532-0	1.543-0	1.577-0	1.513-0	1.540-0	1.540-0	1.592-0	1.672-0	1.709-0	1.753-0
9	1.532-0	1.543-0	1.577-0	1.513-0	1.540-0	1.540-0	1.592-0	1.672-0	1.709-0	1.753-0
10	1.532-0	1.543-0	1.577-0	1.513-0	1.540-0	1.540-0	1.592-0	1.672-0	1.709-0	1.753-0
11	1.532-0	1.543-0	1.577-0	1.513-0	1.540-0	1.540-0	1.592-0	1.672-0	1.709-0	1.753-0

Table 120

R-CENTROIDS FOR (D(2) S-R)

V	VV	1	2	3	4	5	6	7	8	9	10	11
1	1.374-0	1.381-0	1.434-0	1.414-0	1.435-0	1.450-0	1.450-0	1.487-0	1.500-0	1.517-0	1.534-0	1.553-0
2	1.362-0	1.362-0	1.337-0	1.412-0	1.427-0	1.443-0	1.458-0	1.474-0	1.491-0	1.507-0	1.525-0	1.542-0
3	1.352-0	1.371-0	1.390-0	1.435-0	1.420-0	1.435-0	1.451-0	1.465-0	1.482-0	1.498-0	1.515-0	1.530-0
4	1.350-0	1.371-0	1.344-0	1.393-0	1.413-0	1.424-0	1.443-0	1.458-0	1.474-0	1.490-0	1.503-0	1.537-0
5	1.350-0	1.364-0	1.370-0	1.393-0	1.407-0	1.422-0	1.437-0	1.451-0	1.466-0	1.481-0	1.509-0	1.514-0
6	1.345-0	1.354-0	1.373-0	1.387-0	1.411-0	1.415-0	1.430-0	1.444-0	1.458-0	1.495-0	1.494-0	1.504-0
7	1.335-0	1.343-0	1.362-0	1.381-0	1.395-0	1.410-0	1.424-0	1.438-0	1.439-0	1.473-0	1.486-0	1.493-0
8	1.331-0	1.344-0	1.354-0	1.370-0	1.390-0	1.404-0	1.418-0	1.430-0	1.454-0	1.465-0	1.479-0	1.485-0
9	1.327-0	1.341-0	1.354-0	1.371-0	1.345-0	1.399-0	1.412-0	1.414-0	1.445-0	1.458-0	1.471-0	1.499-0
10	1.323-0	1.337-0	1.350-0	1.363-0	1.376-0	1.389-0	1.398-0	1.421-0	1.433-0	1.446-0	1.471-0	1.480-0
11	1.320-0	1.333-0	1.346-0	1.359-0	1.372-0	1.385-0	2.142-0	1.415-0	1.428-0	1.438-0	1.462-0	1.474-0
12	1.317-0	1.331-0	1.343-0	1.356-0	1.369-0	1.381-0	1.404-0	1.412-0	1.424-0	1.433-0	1.456-0	1.469-0
13	1.315-0	1.321-0	1.341-0	1.353-0	1.366-0	1.377-0	1.398-0	1.418-0	1.420-0	1.446-0	1.452-0	1.464-0
14	1.312-0	1.325-0	1.334-0	1.351-0	1.364-0	1.373-0	1.394-0	1.415-0	1.416-0	1.439-0	1.449-0	1.460-0
15	1.311-0	1.324-0	1.336-0	1.349-0	1.352-0	1.367-0	1.392-0	1.413-0	1.412-0	1.435-0	1.446-0	1.454-0
16	1.309-0	1.322-0	1.335-0	1.348-0	1.350-0	1.357-0	1.390-0	1.411-0	1.407-0	1.432-0	1.444-0	1.443-0
17	1.308-0	1.321-0	1.334-0	1.347-0	1.359-0	1.312-0	1.348-0	1.398-0	1.400-0	1.431-0	1.442-0	1.437-0
18	1.307-0	1.321-0	1.333-0	1.346-0	1.358-0	1.441-0	1.347-0	1.398-0	1.396-0	1.429-0	1.440-0	1.487-0
19	1.307-0	1.311-0	1.332-0	1.345-0	1.357-0	1.394-0	1.346-0	1.367-0	1.340-0	1.424-0	1.439-0	1.472-0
20	1.306-0	1.311-0	1.332-0	1.344-0	1.356-0	1.393-0	1.335-0	1.367-0	2.023-0	1.429-0	1.439-0	1.467-0

NOT REPRODUCIBLE

Table 120 (cont'd)

(O(2) 5-2)

	12	13	14	15	16	17	18	19	20	21	22	23
1	1.572-0	1.591-0	1.612-0	1.634-0	1.657-0	1.680-0	1.704-0	1.729-0	1.755-0	1.783-0	1.810-0	1.835-0
2	1.553-0	1.573-0	1.594-0	1.617-0	1.640-0	1.664-0	1.689-0	1.715-0	1.743-0	1.771-0	1.799-0	1.826-0
3	1.443-0	1.472-0	1.502-0	1.532-0	1.562-0	1.594-0	1.627-0	1.661-0	1.696-0	1.731-0	1.765-0	1.799-0
4	1.533-0	1.564-0	1.594-0	1.624-0	1.654-0	1.684-0	1.714-0	1.744-0	1.774-0	1.804-0	1.834-0	1.864-0
5	1.522-0	1.557-0	1.592-0	1.627-0	1.662-0	1.697-0	1.732-0	1.767-0	1.802-0	1.837-0	1.872-0	1.907-0
6	1.532-0	1.567-0	1.602-0	1.637-0	1.672-0	1.707-0	1.742-0	1.777-0	1.812-0	1.847-0	1.882-0	1.917-0
7	1.516-0	1.551-0	1.586-0	1.621-0	1.656-0	1.691-0	1.726-0	1.761-0	1.796-0	1.831-0	1.866-0	1.901-0
8	1.516-0	1.551-0	1.586-0	1.621-0	1.656-0	1.691-0	1.726-0	1.761-0	1.796-0	1.831-0	1.866-0	1.901-0
9	1.449-0	1.484-0	1.519-0	1.554-0	1.589-0	1.624-0	1.659-0	1.694-0	1.729-0	1.764-0	1.799-0	1.834-0
10	1.432-0	1.467-0	1.502-0	1.537-0	1.572-0	1.607-0	1.642-0	1.677-0	1.712-0	1.747-0	1.782-0	1.817-0
11	1.433-0	1.468-0	1.503-0	1.538-0	1.573-0	1.608-0	1.643-0	1.678-0	1.713-0	1.748-0	1.783-0	1.818-0
12	1.432-0	1.467-0	1.502-0	1.537-0	1.572-0	1.607-0	1.642-0	1.677-0	1.712-0	1.747-0	1.782-0	1.817-0
13	1.431-0	1.466-0	1.501-0	1.536-0	1.571-0	1.606-0	1.641-0	1.676-0	1.711-0	1.746-0	1.781-0	1.816-0
14	1.433-0	1.468-0	1.503-0	1.538-0	1.573-0	1.608-0	1.643-0	1.678-0	1.713-0	1.748-0	1.783-0	1.818-0
15	1.479-0	1.514-0	1.549-0	1.584-0	1.619-0	1.654-0	1.689-0	1.724-0	1.759-0	1.794-0	1.829-0	1.864-0
16	1.478-0	1.513-0	1.548-0	1.583-0	1.618-0	1.653-0	1.688-0	1.723-0	1.758-0	1.793-0	1.828-0	1.863-0
17	1.474-0	1.509-0	1.544-0	1.579-0	1.614-0	1.649-0	1.684-0	1.719-0	1.754-0	1.789-0	1.824-0	1.859-0
18	1.472-0	1.507-0	1.542-0	1.577-0	1.612-0	1.647-0	1.682-0	1.717-0	1.752-0	1.787-0	1.822-0	1.857-0
19	1.471-0	1.506-0	1.541-0	1.576-0	1.611-0	1.646-0	1.681-0	1.716-0	1.751-0	1.786-0	1.821-0	1.856-0
20	1.471-0	1.506-0	1.541-0	1.576-0	1.611-0	1.646-0	1.681-0	1.716-0	1.751-0	1.786-0	1.821-0	1.856-0

APPENDIX IV

ADDITIONAL TABLES FOR BIRGE-HOPFIELD TABLES

The purpose of this appendix is to supplement data appearing in the main text of this technical report. New data has been published and these data have been incorporated into the tables of Franck-Condon factors included in this report. To minimize the changes to the main body of the report, these data are being included in this appendix.

The confusing and contradictory tangle of excited states for the very high energies in the nitrogen molecule has been unraveled (Refs. 41, 42, 43). Dressler (Ref. 41) reports that the former twenty states of excited nitrogen can be regrouped into three valence states and three Rydberg states. The three valence states are the $b^1\pi_u$, $b'^1\Sigma_u^+$, and d' . It will be noted that the first two states are those associated with the Birge-Hopfield band systems which are pertinent to this report. The renumbering of the levels of these states has vastly increased the number of vibrational levels for the upper states of each of these systems. This necessitated recalculating the vibrational transition probabilities. The input data used to calculate the vibrational potential for the $b'^1\Sigma$ state was the deperturbed spectroscopic constants of Dressler. These data are listed in table 121. For the input data needed for the $b^1\pi$ state, the data given by Carroll and Collins was graphically smoothed and used. These smoothed data are listed in table 122. The potentials resulting from these data are listed in tables 123 and 124. The potentials were generated using program TURNPT. The vibrational transition probabilities were calculated using program FRANKON. The Franck-Condon factors are listed in tables 60 and 61.

Table 121

SPECTROSCOPIC CONSTANTS FOR THE $N_2b'^1\Sigma_u^+$ STATE

\underline{v}	$\underline{G_v}$	$\underline{B_v}$
0	371.9	1.151
1	1112.0	1.143
2	1848.0	1.135
3	2580.0	1.127
4	3308.0	1.119
5	4031.0	1.111
6	4750.0	1.103
7	5464.0	1.095
8	6174.0	1.087
9	6879.0	1.079
10	7580.0	1.071
11	8276.0	1.063
12	8960.0	1.055
13	9632.0	1.047
14	10292.0	1.039
15	10940.0	1.031
16	11576.0	1.023
17	12200.0	1.015
18	12812.0	1.007
19	13412.0	0.999
20	14099.0	0.991

Table 122

POTENTIAL ENERGY FOR THE $N_2b'^1\Sigma_u^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	371.9	1.3672	1.5282	0.0461
1	1112.0	1.3158	1.5953	0.1380
2	1848.0	1.2825	1.6443	0.2292
3	2580.0	1.2568	1.6859	0.3199
4	3308.0	1.2355	1.7231	0.4102
5	4031.0	1.2170	1.7576	0.4999
6	4750.0	1.2007	1.7899	0.5890
7	5464.0	1.1861	1.8207	0.6775
8	6174.0	1.1729	1.8501	0.7655
9	6879.0	1.1607	1.8786	0.8529
10	7580.0	1.1495	1.9061	0.9398
11	8276.0	1.1389	1.9333	1.0261
12	8960.0	1.1283	1.9612	1.1109
13	9632.0	1.1181	1.9889	1.1942
14	10292.0	1.1083	2.0167	1.2761
15	10940.0	1.0988	2.0445	1.3564
16	11576.0	1.0896	2.0723	1.4352
17	12200.0	1.0807	2.1001	1.5126
18	12812.0	1.0719	2.1283	1.5885
19	13412.0	1.0640	2.1552	1.6629
20	14099.0	1.0701	2.1504	1.7480

Table 123

POTENTIAL ENERGY FOR THE $N_2b^1\pi_u$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	313.2	1.2053	1.3819	0.0388
1	947.0	1.1553	1.4540	0.1174
2	1632.0	1.1288	1.5031	0.2024
3	2354.0	1.1090	1.5445	0.2918
4	3110.0	1.0969	1.5792	0.3856
5	3889.0	1.0859	1.6121	0.4822
6	4682.0	1.0765	1.6437	0.5805
7	5481.0	1.0687	1.6751	0.6794
8	6278.0	1.0616	1.7063	0.7784
9	7063.0	1.0550	1.7390	0.8757
10	7831.0	1.0490	1.7725	0.9708
11	8578.0	1.0432	1.8070	1.0635
12	9303.0	1.0382	1.8426	1.1533
13	10004.0	1.0337	1.8794	1.2403
14	10682.0	1.0298	1.9169	1.3243
15	11337.0	1.0263	1.9555	1.4055
16	11967.0	1.0231	1.9954	1.4836
17	12575.0	1.0206	2.0359	1.5590
18	13159.0	1.0182	2.0780	1.6314
19	13719.0	1.0162	2.1216	1.7009
20	14255.0	1.0150	2.1672	1.7673
21	14768.0	1.0147	2.2149	1.8309
22	15257.0	1.0135	2.2652	1.8915

Table 124

SPECTROSCOPIC CONSTANTS FOR THE $N_2b^1\pi_u$ STATE

\underline{v}	$\underline{G_v}$	$\underline{B_v}$
0	313.2	1.442
1	947.0	1.424
2	1632.0	1.400
3	2354.0	1.376
4	3110.0	1.359
5	3889.0	1.334
6	4682.0	1.313
7	5481.0	1.286
8	6278.0	1.263
9	7063.0	1.235
10	7831.0	1.208
11	8578.0	1.181
12	9303.0	1.150
13	10004.0	1.120
14	10682.0	1.089
15	11337.0	1.059
16	11967.0	1.028
17	12575.0	0.997
18	13159.0	0.966
19	13719.0	0.934
20	14255.0	0.898
21	14768.0	0.860
22	15257.0	0.819

REFERENCES

1. Steele, D., Lippincott, E., Vanderslice, J., "Comparative Study of Empirical Internuclear Potential Functions," Rev. Mod. Phys. 34, 239 (1962).
2. Rydberg, R., Ann. Physik 73, 376 (1931).
3. Klein, O., Z. Physik 76, 226 (1932).
4. Rees, A., Proc. Phys. Soc. (London) A59, 998 (1947).
5. Vanderslice, J., Mason, E., Maisch, W., Lippincott, E., "Ground State of Hydrogen by the Rydberg-Klein-Rees Method," J. Mol. Spectr. 3, 17 (1959).
6. Jarman, W., "Klein-Dunham Potential Energy Functions in Simplified Analytical Form," Can. J. Phy. 38, 217 (1960).
7. Dunham, J., "The Energy Levels of a Rotating Vibrator," Phys. Rev. 41, 721 (1932).
8. Hurley, A., "Equivalence of Rydberg-Klein-Rees and Simplified Dunham Potentials," J. Chem. Phys. 36, 1117 (1962).
9. Ginter, M., Battino, R., "On the Calculation of Potential Curves by the Rydberg-Klein-Rees Method I. Experimental Limitations, Extrapolation Procedures, and Applications to the Third-Group Hydrides," J. Chem. Phys. 42, 200 (1965).
10. Kasper, J. (mentioned in Ref. 12).
11. Cooley, J., Math. Computation 15, 363 (1961) (mentioned in Ref. 12).
12. Zare, R., "Calculation of Intensity Distribution in the Vibrational Structure of Electronic Transitions: The $B^3\Pi_0^+ - X^1\Sigma_0^+$ Resonance Series of Molecular Iodine," J. Chem. Phys. 40, 1934 (1964).
13. Fallon, R., Vanderslice, J., Cloney, R., "Potential Curves and Rotational Perturbations of CN," J. Chem. Phys. 37, 1097 (1962).
14. Nicholls, R., "Franck-Condon Factors to High Vibrational Quantum IV: CN," J. Res. NBS 68A, 75 (1964).
15. Spindler, R., Franck-Condon Factors Based on RKR Potentials with Applications to Radiative Absorption Coefficients, Avco TM 64-55, 30 September 1964.
16. Krupenie, P., Weissman, S., "Potential Energy Curves for CO and CO^+ ," J. Chem. Phys. 43, 1529 (1965).
17. Nicholls, R., "Laboratory Astrophysics," J. Q. S. R. T. 2, 433 (1962).

REFERENCES (cont'd)

18. Benesch, W., Vanderslice, J., Tilford, S., Wilkinson, P., "Potential Curves for the Observed States of N_2 Below 11 ev," Astrophys. J. 142, 1227 (1965).
19. Lofthus, A., "The Molecular Spectrum of Nitrogen," Spectroscopic Report Number 2, Department of Physics, University of Oslo, December 1960.
20. Wilkinson, P., Houk, N., "Emission Spectra of Nitrogen in the Vacuum Ultraviolet," J. Chem. Phys. 24, 528 (1956).
21. Gilmore, F., Thermal Radiation Phenomenon, DASA-1971, Vol 1 (1967).
22. Vanderslice, J., Mason, E., Maisch, W., "Interactions between Oxygen and Nitrogen: $O-N$, $O-N_2$, O_2-N_2 ," J. Chem. Phys. 31, 738 (1959).
23. Vanderslice, J., "Modification of the Rydberg-Klein-Rees Method for Obtaining Potential Curves, Doublet States Intermediate between Hund's Cases (a) and (b)," J. Chem. Phys. 37, 384 (1962).
24. Wallace, L., "Band-Head Wavelengths of C_2 , CH , CN , CO , NH , NO , NO_2 , OH , and Their Ions," Astrophysical Journal Supplement Series No. 68, Vol VII, 165, October 1962.
25. Vanderslice, J., Mason, E., Maisch, M., Lippincott, E., "Potential Curves for N_2 , NO , and O_2 ," J. Chem. Phys. 33, 614 (1960).
26. Gilmore, F., RAND Corporation, private communication.
27. Richards, W., Barrow, R., "The Calculation of Potential Curves for Diatomic Molecules from Experimental Data," Proc. Phy. Soc. 83, 1045 (1964).
28. Ginter, M., Battino, R., "On the Calculation of Potential Curves by the Rydberg-Klein-Rees Method I. Experimental Limitations, Extrapolation Procedures, and Applications to the Third-Group Hydrides," J. Chem. Phys. 42, 3222 (1965).
29. Halmann, M., Laulicht, I., "Isotope Effects on Franck-Condon Factors, VII, Vibrational Intensity Distribution in the H_2 Lyman, H_2 Werner, O_2 Schumann-Runge, N_2 First Positive, N_2 Vegard-Kaplan, and LiH (A-X) Systems Based on RKR Potentials," J. Chem. Phys. 46, 2684 (1967).
30. Evans, J., Schexander, C., An Investigation of the Effect of High Temperature on the Schumann-Runge Ultraviolet Absorption Continuum of Oxygen, NASA TR R-92 (1961).
31. Herzberg, G., Molecular Spectra and Molecular Structure, I, Spectra of Diatomic Molecules, Van Nostrand (1950).
32. Miescher, E., "Spectrum and Energy Levels at the NO Molecule," J. Q. S. R. T. 2, 421 (1966).

REFERENCES (cont'd)

33. Air Force Weapons Laboratory material unpublished before this report, Kirtland AFB, New Mexico.
34. Jain, D., Sahni, R., "Transition Probability Parameters of the Band Systems of CO^+ ," J. Q. S. R. T. 6, 705 (1966).
35. Jain, D., Sahni, R., "Variation of Electronic Transition Moment in Some Band Systems of the N_2 Molecule," J. Q. S. R. T. 7, 475 (1967).
36. Benesch, W., Vanderslice, J., Tilford, S., Wilkinson, G., "Franck-Condon Factors for Permitted Transitions in N_2 ," Ap. J. 144, 408 (1965).
37. Zare, R., Larsson, E., Berg, R., "Franck-Condon Factors for Electronic Band Systems of Molecular Nitrogen," J. Mol. Spectr. 15, 117 (1965).
38. Flinn, D., Spindler, R., Fifer, S., Kelly, M., "Franck-Condon Factors for the β and γ Bands of the NO Molecule Based on Realistic Potential Functions," J. Q. S. R. T. 4, 271 (1964).
39. Jarman, W., "Franck-Condon Factors from Klein-Dunham Potentials for Bands of the Schumann-Runge System of O_2 ," Can. J. Phys. 41, 414 (1963).
40. Wallace, L., "Emission Band Spectra of Nitrogen," Ap. J. Suppl. 6, 445 (1962).
41. Dressler, K., "The Lowest Valence and Rydberg States in the Dipole Allowed Absorption Spectrum of Nitrogen. A Survey of Their Interactions," Can. J. Phys., 47, 547 (1969).
42. Carroll, P., Collins, C., "High Resolution Absorption Studies of the $b^1\pi_u + X^1\Sigma_g^+$ System of Nitrogen," Can. J. Phys., 47, 563 (1969).
43. Lefebvre-Brion, H., "Theoretical Study of Homogeneous Perturbations, II. Least-Squares Fitting Method to Obtain 'Deperturbed' Crossing Morse Curves. Application to the Perturbed $1\Sigma_u^+$ States of N_2 ," Can. J. Phys., 47, 543 (1969).

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